



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 01:54 AM UTC

PDB ID : 6XBW / pdb_00006xbw
EMDB ID : EMD-22121
Title : Cryo-EM structure of V-ATPase from bovine brain, state 1
Authors : Wang, R.; Li, X.
Deposited on : 2020-06-07
Resolution : 3.37 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

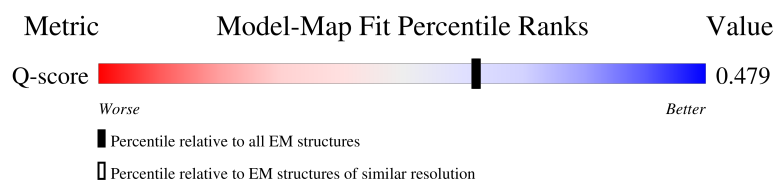
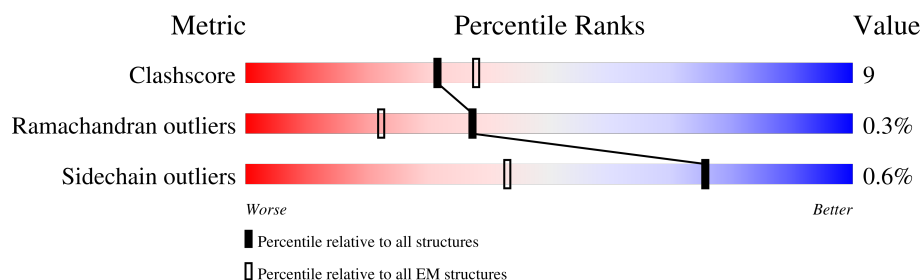
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



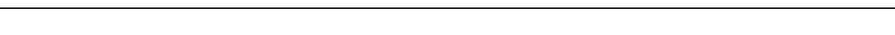
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14287 (2.87 - 3.87)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
2	D	511	

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Mol	Chain	Length	Quality of chain
2	E	511	
2	F	511	
3	G	382	
4	H	247	
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	P	465	
9	a	838	
10	b	205	
11	d	351	
12	e	81	
13	s	468	
14	r	351	
15	c	155	
15	g	155	
15	k	155	
15	l	155	
15	m	155	
15	n	155	
15	o	155	

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Mol	Chain	Length	Quality of chain
15	p	155	
15	q	155	
16	f	98	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	NAG	s	506	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 63090 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	589	Total	C	N	O	S	0	0
			4568	2900	770	870	28		
1	B	590	Total	C	N	O	S	0	0
			4582	2906	773	876	27		
1	C	597	Total	C	N	O	S	0	0
			4628	2935	781	884	28		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	461	Total	C	N	O	S	0	0
			3609	2288	618	683	20		
2	E	458	Total	C	N	O	S	0	0
			3585	2273	613	679	20		
2	F	459	Total	C	N	O	S	0	0
			3594	2279	615	680	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	346	Total	C	N	O	S	0	0
			2823	1820	475	519	9		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	211	Total	C	N	O	S	0	0
			1700	1080	307	308	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1614	1009	296	302	7		
5	J	218	Total	C	N	O	S	0	0
			1624	1018	297	302	7		
5	K	220	Total	C	N	O	S	0	0
			1595	994	297	298	6		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	103	Total	C	N	O	S	0	0
			816	516	143	156	1		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	108	Total	C	N	O	S	0	0
			665	395	138	129	3		
7	N	108	Total	C	N	O	S	0	0
			665	395	138	129	3		
7	O	108	Total	C	N	O	S	0	0
			665	395	138	129	3		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	368	Total	C	N	O	S	0	0
			2819	1783	498	522	16		

- Molecule 9 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	750	Total	C	N	O	S	0	0
			6093	3979	1013	1062	39		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	204	Total	C	N	O	S	0	0
			1503	996	238	259	10		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	348	Total	C	N	O	S	0	0
			2819	1817	460	528	14		

- Molecule 12 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	73	Total	C	N	O	S	0	0
			590	409	91	87	3		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	205	Total	C	N	O	S	0	0
			1668	1083	264	312	9		

- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	46	Total	C	N	O	S	0	0
			385	261	54	67	3		

- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	g	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	k	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	l	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	m	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	n	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	o	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
15	p	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
15	q	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		

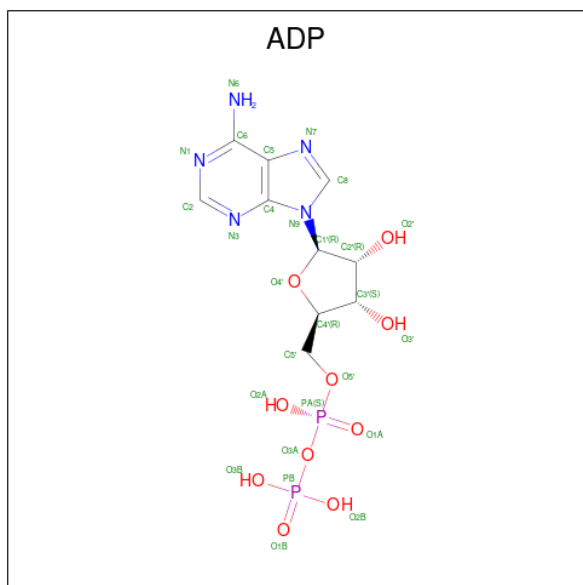
- Molecule 16 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	45	Total	C	N	O	S	0	0
			351	240	52	55	4		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

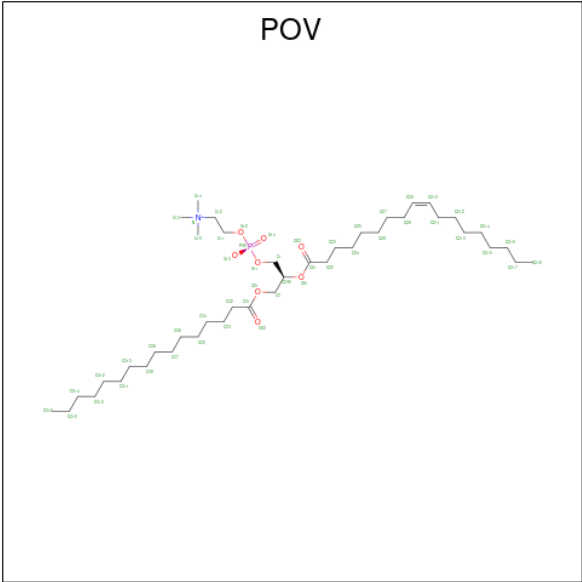
Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Mg	0
			1	1	

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



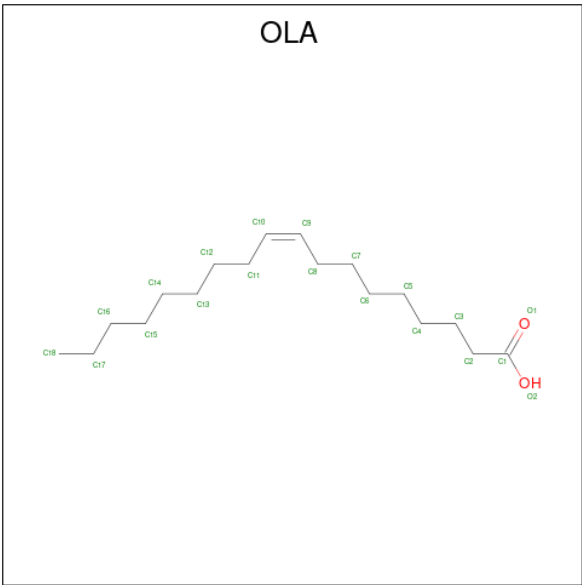
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			31	21	1	8	1	
19	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
19	p	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 20 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 21 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).

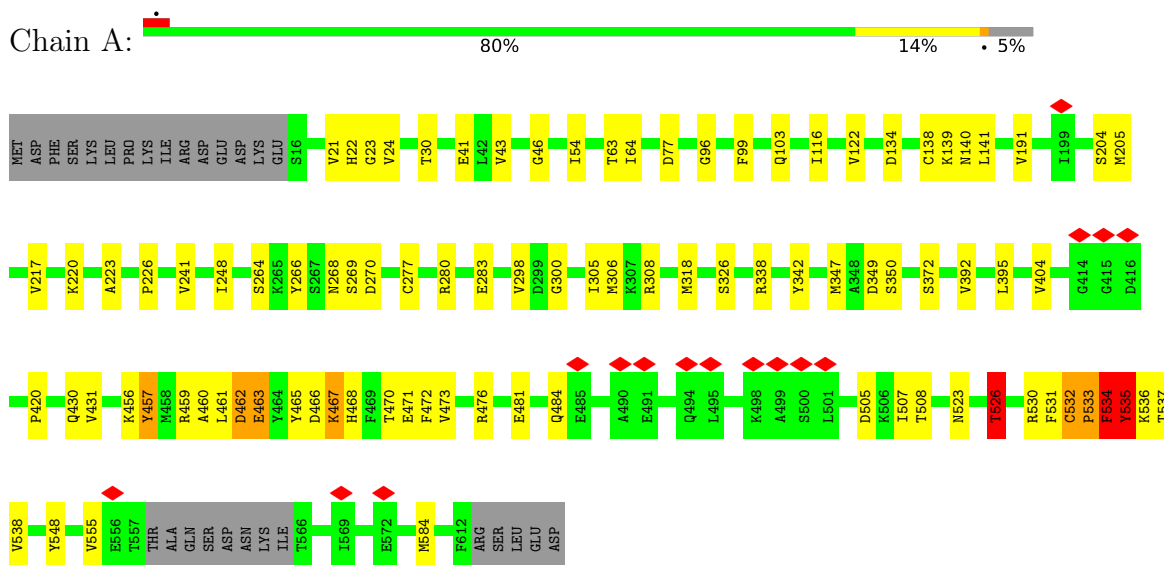


Mol	Chain	Residues	Atoms			AltConf
21	r	1	Total	C	O	0
			20	18	2	

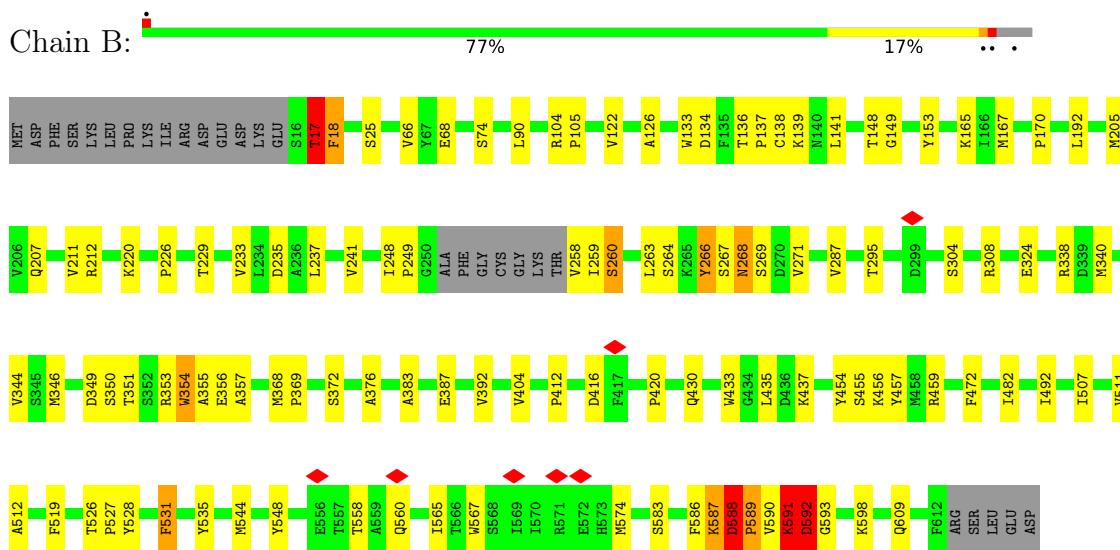
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: V-type proton ATPase catalytic subunit A



- Molecule 1: V-type proton ATPase catalytic subunit A



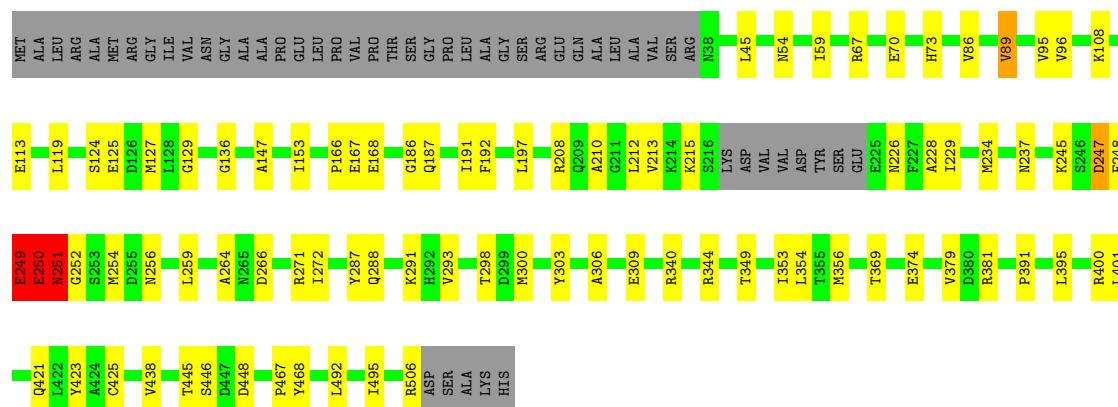
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain C:  81% 15% . .



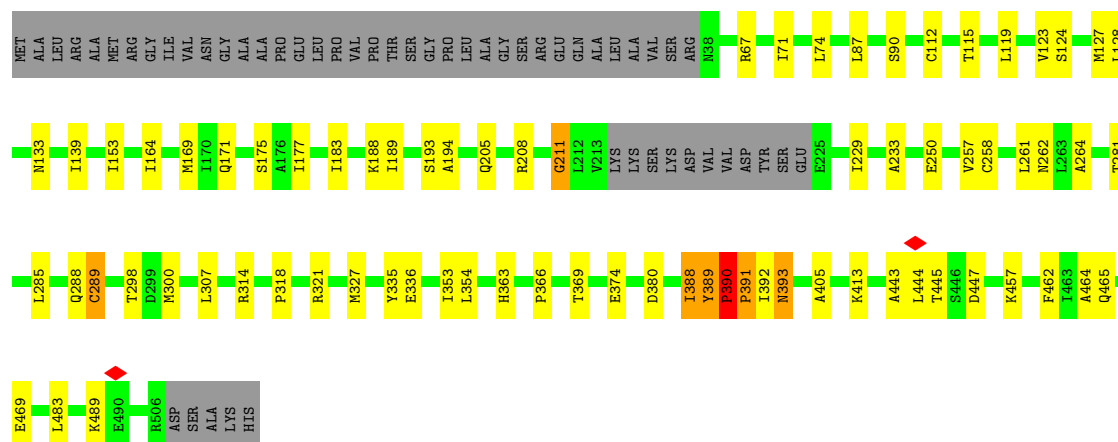
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:  73% 16% . 10%



- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E:  75% 13% . 10%



- Molecule 2: V-type proton ATPase subunit B, brain isoform

LVS	HIS	Met
R271	T274	ALA
L285	L285	ALA
C289	C289	ALA
T298	T298	ALA
D299	D299	ALA
M300	M300	ALA
R340	R340	ALA
T349	T349	ALA
L354	L354	ALA
T355	T355	ALA
V379	V379	ALA
I388	I388	ALA
L395	L395	ALA
R400	R400	ALA
D414	D414	ALA
Y423	Y423	ALA
M435	M435	ALA
A436	A436	ALA
V438	V438	ALA
V439	V439	ALA
E442	E442	ALA
A443	A443	ALA
L444	L444	ALA
T445	T445	ALA
A464	A464	ALA
W481	W481	ALA
R485	R485	ALA
P498	P498	ALA
M491	M491	ALA
S498	S498	ALA
S501	S501	ALA
B506	B506	ALA
ASP	ASP	ALA
SER	SER	ALA
E125	E125	ALA
D126	D126	ALA
R130	R130	ALA
V131	V131	ALA
F132	F132	ALA
M133	M133	ALA
K137	K137	ALA
P138	P138	ALA
I139	I139	ALA
P143	P143	ALA
A147	A147	ALA
I164	I164	ALA
T172	T172	ALA
D178	D178	ALA
I183	I183	ALA
G186	G186	ALA
I189	I189	ALA
S193	S193	ALA
R214	R214	ALA
LYS	LYS	ALA
SER	SER	ALA
LYS	LYS	ALA
ASP	ASP	ALA
VAL	VAL	ALA
ASP	ASP	ALA
TTR	TTR	ALA
SER	SER	ALA
GLU	GLU	ALA
E225	E225	ALA
A233	A233	ALA
M234	M234	ALA
R242	R242	ALA
E249	E249	ALA
M254	M254	ALA
L259	L259	ALA
P260	P260	ALA
L261	L261	ALA
N262	N262	ALA
T268	T268	ALA
I269	I269	ALA
E270	E270	ALA
E125	E125	ALA
D126	D126	ALA
R130	R130	ALA
V131	V131	ALA
F132	F132	ALA
M133	M133	ALA
K137	K137	ALA
P138	P138	ALA
I139	I139	ALA
P143	P143	ALA
A147	A147	ALA
I164	I164	ALA
T172	T172	ALA
D178	D178	ALA
I183	I183	ALA
G186	G186	ALA
I189	I189	ALA
S193	S193	ALA
R214	R214	ALA
LYS	LYS	ALA
SER	SER	ALA
LYS	LYS	ALA
ASP	ASP	ALA
VAL	VAL	ALA
ASP	ASP	ALA
TTR	TTR	ALA
SER	SER	ALA
GLU	GLU	ALA
E225	E225	ALA
A233	A233	ALA
M234	M234	ALA
R242	R242	ALA
E249	E249	ALA
M254	M254	ALA
L259	L259	ALA
P260	P260	ALA
L261	L261	ALA
N262	N262	ALA
T268	T268	ALA
I269	I269	ALA
E270	E270	ALA
E125	E125	ALA
D126	D126	ALA
R130	R130	ALA
V131	V131	ALA
F132	F132	ALA
M133	M133	ALA
K137	K137	ALA
P138	P138	ALA
I139	I139	ALA
P143	P143	ALA
A147	A147	ALA
I164	I164	ALA
T172	T172	ALA

Chain G: 76% 14% 9%

K326	K330	S344	SER	ALA	ALA	ALA	ILE	ILE	ASP	ALA	PRO	MET	ASP	ILE	PRO	GLY	LEU	ASN	LEU	SER	GLN	GLN	GLU	Y366	L379	GLU	PHE	LYS	L118	K119	N120	E123	K137	L150	L153	D178	S179	E180	V187	E218	S222	Y223	A241	F246	I247	V248	N254	E255	D261	K262	E263	E264	M265	N266	R267	L268	S269	D271	K272	K273	K274	P278	R281	R301	Y310	Q317	L320	MET	T2	E3	F4	P10	G11	GLU	LYS	THR	CYS	GLN	GLN	T18	K21	L22	H23	T26	T27	N30	N31	L32	S35	F38	D42	T47	L48	D49	V50	L51	L54	S55	D56	D62	V63	K71	L80	GLU	ASP	SER	LYS	ASP	R86	N94	Q116
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Chain H: 65% 19% • 15%

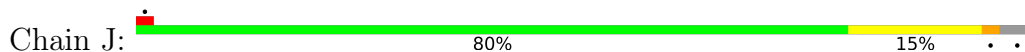
[illegible]

Chain I: 5% 86% 10%

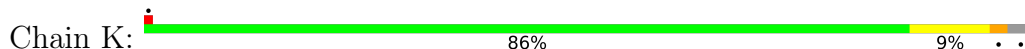
Protein	Number of Amino Acids
NET	195
ALA	190
LEU	185
SER	180
ASP	175
A6	170
K26	165
E29	160
I30	155
D31	150
A32	145
K33	140
A34	135
E35	130
E36	125
E37	120
I40	115
E55	110
E58	105
L81	100
R85	95
D93	90
N96	85
L116	80
Q122	75
V144	70
Y155	65
R161	60
D162	55
V163	50
D164	45
V165	40
E176	35
G180	30
I183	25
V192	20
T195	15
L202	10
C206	5



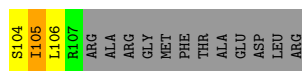
- Molecule 5: V-type proton ATPase subunit E 1



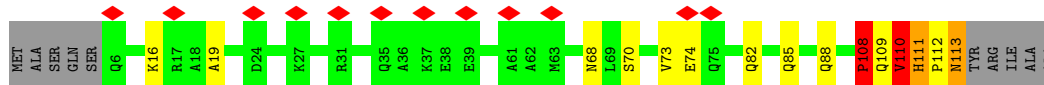
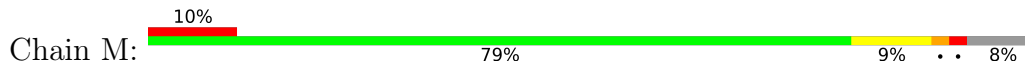
- Molecule 5: V-type proton ATPase subunit E 1



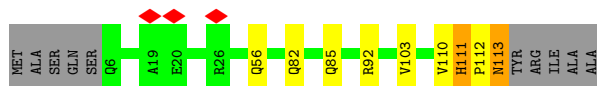
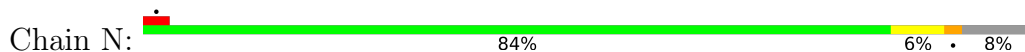
- Molecule 6: V-type proton ATPase subunit F



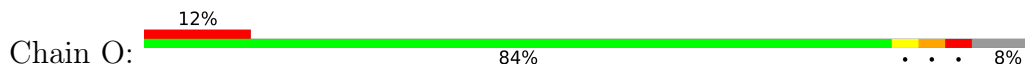
- Molecule 7: V-type proton ATPase subunit G

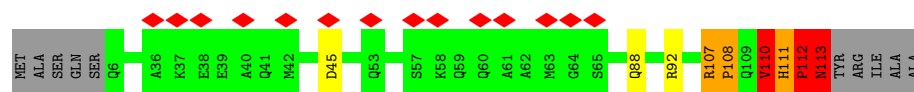


- Molecule 7: V-type proton ATPase subunit G



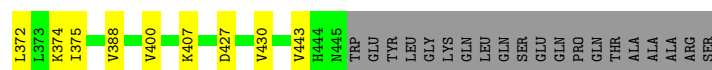
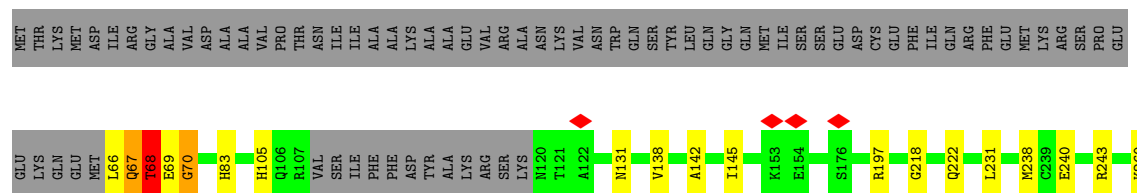
- Molecule 7: V-type proton ATPase subunit G





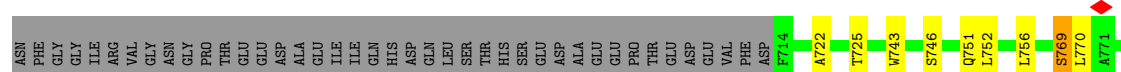
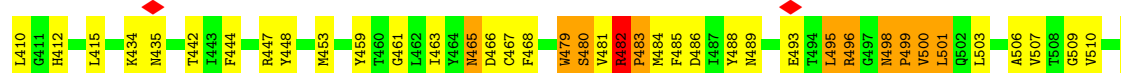
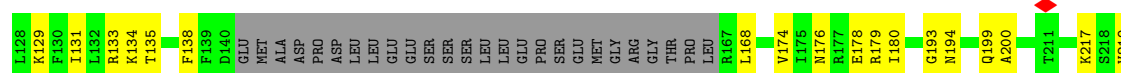
- Molecule 8: V-type proton ATPase subunit H

Chain P: 64% 13% 21%



- Molecule 9: V-type proton ATPase subunit a

Chain a: 69% 18% 11%



- Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit

18%



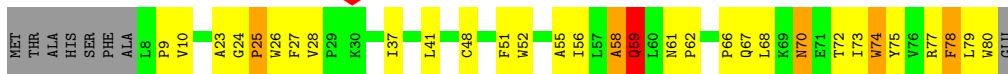
- Molecule 11: V-type proton ATPase subunit d 1

17%



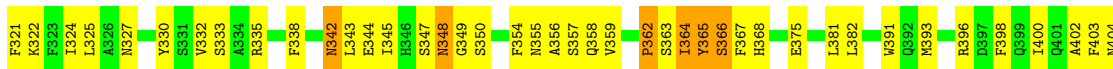
- Molecule 12: V-type proton ATPase subunit e 2

10%



- Molecule 13: V-type proton ATPase subunit S1

56%





- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain m: 85% 12%



- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain n: 81% 15%



- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain o: 86% 12%



- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain p: 86% 10%



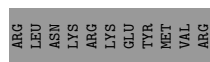
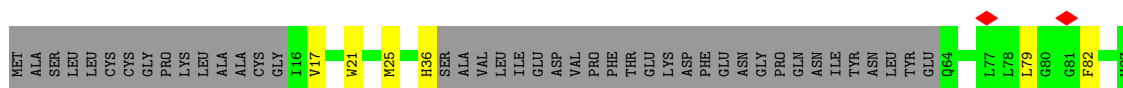
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain q: 83% 15%



- Molecule 16: Ribonuclease kappa

Chain f: 40% 6% 54%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84345	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	31.875	Depositor
Minimum map value	-17.506	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.129	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	424.83002, 424.83002, 424.83002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.833, 0.833, 0.833	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: POV, ADP, OLA, NAG, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	21/4663 (0.5%)	0.89	28/6314 (0.4%)
1	B	1.00	44/4676 (0.9%)	1.00	32/6333 (0.5%)
1	C	0.60	16/4724 (0.3%)	0.74	18/6398 (0.3%)
2	D	0.53	9/3680 (0.2%)	0.84	11/4986 (0.2%)
2	E	0.38	2/3656 (0.1%)	0.76	19/4956 (0.4%)
2	F	0.21	0/3665	0.61	5/4967 (0.1%)
3	G	0.20	0/2875	0.63	4/3883 (0.1%)
4	H	0.55	3/1718 (0.2%)	0.74	5/2298 (0.2%)
5	I	0.39	2/1627 (0.1%)	0.71	2/2196 (0.1%)
5	J	0.58	2/1637 (0.1%)	0.61	3/2208 (0.1%)
5	K	0.52	4/1606 (0.2%)	0.72	6/2171 (0.3%)
6	L	1.03	9/829 (1.1%)	1.40	19/1122 (1.7%)
7	M	0.91	7/667 (1.0%)	1.22	12/912 (1.3%)
7	N	0.96	10/667 (1.5%)	0.93	9/912 (1.0%)
7	O	0.97	6/667 (0.9%)	1.16	7/912 (0.8%)
8	P	0.30	1/2865 (0.0%)	0.97	24/3877 (0.6%)
9	a	0.39	4/6246 (0.1%)	0.80	38/8451 (0.4%)
10	b	0.79	9/1537 (0.6%)	0.67	7/2090 (0.3%)
11	d	0.21	0/2884	0.71	8/3906 (0.2%)
12	e	0.90	2/613 (0.3%)	1.27	9/844 (1.1%)
13	s	1.00	16/1720 (0.9%)	1.22	26/2341 (1.1%)
14	r	1.42	8/398 (2.0%)	0.93	2/547 (0.4%)
15	c	0.19	0/1079	0.51	0/1459
15	g	0.17	0/1079	0.44	0/1459
15	k	0.17	0/1079	0.48	0/1459
15	l	0.17	0/1079	0.46	0/1459
15	m	0.17	0/1079	0.47	0/1459
15	n	0.18	0/1079	0.47	0/1459
15	o	0.18	0/1088	0.47	1/1470 (0.1%)
15	p	0.17	0/1088	0.46	1/1470 (0.1%)
15	q	0.18	0/1088	0.58	1/1470 (0.1%)
16	f	0.21	0/359	0.61	1/485 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.59	175/63717 (0.3%)	0.80	298/86273 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
2	D	0	1
5	I	0	1
7	M	0	1
7	N	0	1
8	P	0	1
9	a	0	1
13	s	0	1
All	All	0	12

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	TYR	C-O	-24.28	0.93	1.24
1	A	535	TYR	CA-C	-22.23	1.22	1.52
1	B	592	ASP	C-O	-20.20	0.98	1.24
13	s	305	ALA	C-N	19.28	1.57	1.33
1	A	535	TYR	N-CA	-18.93	1.22	1.46
1	A	535	TYR	CE1-CZ	-18.07	0.94	1.38
1	A	534	PHE	C-O	-16.92	1.03	1.24
1	A	535	TYR	CZ-OH	-16.65	1.03	1.38
1	B	592	ASP	CA-C	-16.59	1.30	1.52
1	B	593	GLY	C-O	-15.76	1.02	1.23
1	B	137	PRO	N-CD	-15.71	1.25	1.47
10	b	22	VAL	C-N	15.42	1.56	1.33
2	E	388	ILE	C-N	14.55	1.54	1.33
5	J	153	PRO	N-CD	-14.39	1.27	1.47
2	D	247	ASP	CA-C	-13.43	1.40	1.53
9	a	483	PRO	N-CD	-13.37	1.29	1.47
1	B	455	SER	CA-CB	-12.00	1.32	1.53
7	N	111	HIS	CA-C	-11.68	1.38	1.52
1	C	456	LYS	CA-C	-10.98	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	112	PRO	C-O	-10.74	1.09	1.24
14	r	329	ILE	C-O	-10.50	1.13	1.24
1	A	535	TYR	CG-CD2	-10.44	1.17	1.39
1	B	456	LYS	CA-C	-10.44	1.39	1.52
1	B	456	LYS	C-O	-10.12	1.10	1.24
1	A	534	PHE	CG-CD2	-9.67	1.18	1.38
14	r	330	TRP	C-O	-9.52	1.12	1.24
6	L	98	TYR	CA-C	9.21	1.63	1.52
1	B	355	ALA	C-O	-9.19	1.13	1.24
1	B	457	TYR	C-O	-9.05	1.12	1.24
13	s	364	ILE	CA-CB	-8.92	1.43	1.54
1	A	534	PHE	CG-CD1	-8.89	1.20	1.38
7	O	108	PRO	N-CD	-8.89	1.35	1.47
1	B	456	LYS	CA-CB	-8.82	1.40	1.53
1	B	592	ASP	CB-CG	-8.76	1.30	1.52
1	C	456	LYS	C-O	-8.61	1.12	1.24
13	s	357	SER	C-N	-8.53	1.21	1.33
1	B	457	TYR	CZ-OH	-8.41	1.20	1.38
1	C	456	LYS	CA-CB	-8.40	1.40	1.53
1	B	354	TRP	C-O	-8.35	1.14	1.24
7	M	112	PRO	C-O	-8.28	1.13	1.24
13	s	364	ILE	C-O	-8.21	1.14	1.24
2	D	247	ASP	N-CA	-8.18	1.37	1.47
1	B	457	TYR	CB-CG	-8.14	1.33	1.51
1	B	455	SER	C-O	-8.01	1.14	1.23
13	s	417	ALA	CA-C	-7.96	1.42	1.52
7	M	111	HIS	N-CA	-7.92	1.34	1.46
10	b	15	PHE	CA-C	-7.92	1.43	1.52
14	r	325	THR	C-N	7.88	1.44	1.34
2	E	393	ASN	C-N	-7.86	1.25	1.34
1	B	456	LYS	N-CA	-7.84	1.36	1.46
1	C	458	MET	N-CA	-7.79	1.37	1.46
1	B	356	GLU	CA-C	-7.73	1.41	1.52
9	a	517	PHE	C-N	7.71	1.43	1.32
1	B	356	GLU	C-O	-7.68	1.14	1.24
1	A	526	THR	N-CA	-7.66	1.37	1.46
1	C	457	TYR	CZ-OH	-7.61	1.22	1.38
14	r	330	TRP	CA-C	-7.61	1.42	1.52
13	s	365	TYR	C-O	-7.59	1.15	1.23
7	O	112	PRO	CA-CB	-7.58	1.43	1.53
1	C	458	MET	C-O	-7.52	1.14	1.24
1	B	457	TYR	CA-CB	-7.50	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	655	LYS	C-N	7.44	1.40	1.33
1	B	592	ASP	N-CA	7.43	1.55	1.46
1	C	143	VAL	C-N	7.42	1.44	1.33
1	B	350	SER	CA-C	-7.40	1.42	1.52
1	B	353	ARG	CA-CB	-7.38	1.41	1.53
1	B	353	ARG	CA-C	-7.31	1.42	1.52
1	B	592	ASP	CG-OD2	-7.19	1.11	1.25
14	r	328	ASN	CA-C	-7.19	1.42	1.52
10	b	17	ALA	CA-C	-7.18	1.43	1.52
1	B	457	TYR	N-CA	-7.16	1.36	1.46
7	M	111	HIS	CA-CB	-7.14	1.42	1.53
2	D	247	ASP	CA-CB	-7.12	1.44	1.53
5	K	162	ASP	C-O	-7.12	1.16	1.23
1	A	535	TYR	CB-CG	-7.09	1.36	1.51
10	b	17	ALA	C-O	-7.09	1.15	1.24
7	N	111	HIS	N-CA	-7.09	1.36	1.46
1	B	457	TYR	CE1-CZ	-7.03	1.21	1.38
4	H	74	PHE	C-O	-6.97	1.16	1.24
4	H	75	THR	C-O	-6.95	1.15	1.24
7	N	112	PRO	C-O	-6.94	1.15	1.24
1	A	457	TYR	N-CA	-6.93	1.38	1.46
1	C	457	TYR	CB-CG	-6.93	1.36	1.51
2	D	247	ASP	C-O	-6.92	1.18	1.23
10	b	19	LEU	C-O	-6.88	1.16	1.24
1	C	456	LYS	N-CA	-6.88	1.36	1.46
13	s	270	GLN	C-O	-6.88	1.15	1.24
13	s	270	GLN	CA-C	-6.87	1.43	1.52
1	C	457	TYR	C-O	-6.85	1.15	1.23
7	O	112	PRO	N-CA	-6.81	1.38	1.47
7	O	113	ASN	CG-ND2	-6.81	1.19	1.33
1	C	457	TYR	CA-CB	-6.80	1.43	1.52
13	s	363	SER	CA-C	-6.79	1.43	1.52
1	B	357	ALA	C-O	-6.71	1.15	1.24
13	s	417	ALA	C-O	-6.69	1.16	1.24
2	D	250	GLU	C-O	-6.66	1.15	1.24
1	B	356	GLU	CA-CB	-6.63	1.41	1.53
1	A	463	GLU	CA-C	6.62	1.61	1.52
6	L	87	ALA	C-O	-6.58	1.15	1.23
1	B	593	GLY	C-N	-6.56	1.25	1.34
7	M	113	ASN	CG-ND2	-6.56	1.19	1.33
7	O	113	ASN	CG-OD1	-6.56	1.11	1.23
1	B	351	THR	N-CA	-6.48	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	113	ASN	N-CA	-6.45	1.33	1.46
13	s	363	SER	C-O	-6.41	1.15	1.24
10	b	34	ARG	CA-C	-6.41	1.43	1.52
14	r	328	ASN	C-O	-6.39	1.15	1.24
7	N	113	ASN	N-CA	-6.39	1.34	1.46
7	N	112	PRO	CA-CB	-6.38	1.44	1.53
13	s	365	TYR	CA-CB	-6.34	1.43	1.53
1	B	454	TYR	C-N	-6.33	1.25	1.33
6	L	100	ALA	N-CA	6.32	1.54	1.46
7	N	111	HIS	CA-CB	-6.29	1.43	1.53
10	b	41	LEU	C-N	6.19	1.42	1.33
1	A	473	VAL	CA-CB	-6.15	1.51	1.54
7	N	111	HIS	C-O	-6.15	1.16	1.24
1	C	196	PHE	CA-C	-6.10	1.45	1.52
5	J	152	ILE	CA-CB	-6.09	1.46	1.54
1	B	455	SER	CA-C	-6.03	1.45	1.52
2	D	249	GLU	CA-C	-5.98	1.45	1.52
1	A	535	TYR	CA-CB	-5.98	1.43	1.53
9	a	482	ARG	CA-C	-5.96	1.45	1.52
1	B	351	THR	C-O	-5.95	1.15	1.24
4	H	72	ALA	CA-C	-5.93	1.45	1.52
5	K	164	ASP	CA-C	-5.93	1.46	1.53
5	K	163	VAL	CA-CB	-5.92	1.46	1.54
13	s	365	TYR	CA-C	-5.92	1.45	1.53
1	C	136	THR	C-N	5.89	1.41	1.33
8	P	336	GLU	CA-C	-5.85	1.45	1.52
7	N	111	HIS	CB-CG	-5.85	1.42	1.50
1	B	457	TYR	CG-CD1	-5.82	1.27	1.39
14	r	329	ILE	CA-CB	-5.81	1.47	1.54
7	M	111	HIS	CA-C	-5.74	1.45	1.52
10	b	18	CYS	C-O	-5.72	1.16	1.24
1	B	455	SER	CB-OG	-5.72	1.30	1.42
1	A	463	GLU	C-O	-5.71	1.17	1.24
1	B	355	ALA	CA-C	-5.69	1.45	1.52
1	A	532	CYS	CA-C	-5.69	1.46	1.52
1	C	457	TYR	CE1-CZ	-5.67	1.24	1.38
6	L	102	LYS	N-CA	5.64	1.53	1.45
6	L	90	GLU	CA-C	-5.63	1.46	1.52
1	C	17	THR	CA-C	-5.59	1.44	1.52
7	M	112	PRO	CA-CB	-5.56	1.45	1.53
7	N	113	ASN	CG-ND2	-5.56	1.21	1.33
1	B	531	PHE	C-O	-5.54	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	PHE	C-O	-5.51	1.16	1.23
1	B	136	THR	C-N	5.48	1.46	1.33
6	L	103	ASP	C-O	-5.45	1.16	1.24
1	B	593	GLY	CA-C	-5.43	1.44	1.51
12	e	72	THR	C-O	-5.43	1.17	1.24
1	B	455	SER	N-CA	-5.42	1.39	1.45
2	D	251	ASN	CA-CB	-5.42	1.46	1.54
6	L	100	ALA	CA-C	5.42	1.60	1.52
10	b	15	PHE	C-O	-5.40	1.17	1.24
6	L	88	VAL	CA-CB	-5.39	1.47	1.54
13	s	362	PRO	CA-C	-5.36	1.44	1.52
5	K	152	ILE	CA-C	-5.33	1.47	1.52
1	A	457	TYR	CB-CG	-5.33	1.40	1.51
13	s	307	LEU	N-CA	-5.33	1.39	1.46
1	B	354	TRP	CA-C	-5.29	1.46	1.52
5	I	165	VAL	C-O	-5.26	1.17	1.24
1	C	195	GLU	CA-C	-5.25	1.46	1.52
7	N	112	PRO	CA-C	-5.23	1.45	1.52
14	r	329	ILE	CA-C	-5.20	1.46	1.53
5	I	163	VAL	C-O	-5.18	1.18	1.24
1	A	533	PRO	C-N	-5.16	1.26	1.33
2	D	249	GLU	N-CA	-5.16	1.40	1.46
1	A	534	PHE	CA-CB	-5.12	1.45	1.53
1	B	457	TYR	C-N	-5.10	1.26	1.33
1	A	457	TYR	CE1-CZ	-5.10	1.26	1.38
6	L	87	ALA	CA-C	-5.10	1.46	1.52
13	s	308	VAL	CA-CB	-5.06	1.48	1.54
1	B	354	TRP	CB-CG	-5.02	1.34	1.50
12	e	59	GLN	C-O	-5.02	1.17	1.24
2	D	251	ASN	N-CA	-5.01	1.38	1.45

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	212	LEU	N-CA-C	-25.25	73.59	109.95
1	A	534	PHE	N-CA-C	19.38	132.49	111.36
1	B	259	ILE	CB-CA-C	18.45	141.56	111.29
5	I	161	ARG	CB-CA-C	18.37	146.97	110.42
1	B	588	ASP	CA-C-N	17.52	141.75	119.84
1	B	588	ASP	C-N-CA	17.52	141.75	119.84
1	A	535	TYR	CA-C-O	-17.09	100.31	119.97
13	s	417	ALA	N-CA-C	15.98	128.78	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	389	TYR	CA-C-N	15.79	136.65	120.38
2	E	389	TYR	C-N-CA	15.79	136.65	120.38
1	B	591	LYS	O-C-N	-15.67	107.62	123.29
7	M	110	VAL	N-CA-C	-14.73	90.84	108.82
8	P	369	ASN	CA-C-N	14.69	149.59	121.54
8	P	369	ASN	C-N-CA	14.69	149.59	121.54
1	B	260	SER	N-CA-C	14.17	135.26	113.72
2	D	252	GLY	CA-C-N	14.13	143.21	120.60
2	D	252	GLY	C-N-CA	14.13	143.21	120.60
1	A	526	THR	CB-CA-C	14.08	123.11	110.44
13	s	417	ALA	CB-CA-C	-13.57	87.79	110.85
13	s	277	GLY	N-CA-C	-13.54	87.93	110.95
1	B	259	ILE	N-CA-C	-13.50	81.27	109.34
8	P	369	ASN	N-CA-C	13.30	129.75	111.92
7	O	111	HIS	CA-C-N	13.15	136.28	119.84
7	O	111	HIS	C-N-CA	13.15	136.28	119.84
8	P	370	TYR	CA-C-N	12.22	137.65	120.29
8	P	370	TYR	C-N-CA	12.22	137.65	120.29
1	C	199	ILE	N-CA-C	-12.06	91.24	107.88
1	B	591	LYS	CA-C-N	11.98	144.42	121.54
1	B	591	LYS	C-N-CA	11.98	144.42	121.54
6	L	91	ILE	CA-C-N	11.92	132.06	119.78
6	L	91	ILE	C-N-CA	11.92	132.06	119.78
11	d	90	TYR	N-CA-C	-11.76	85.74	110.80
1	C	143	VAL	O-C-N	11.59	135.24	122.61
5	K	163	VAL	CB-CA-C	-11.44	92.52	111.29
2	D	252	GLY	N-CA-C	11.36	131.00	115.32
6	L	99	ASP	N-CA-C	11.32	134.91	110.80
6	L	102	LYS	CA-C-O	11.26	131.27	118.77
12	e	78	PHE	N-CA-C	11.22	126.34	112.87
13	s	364	ILE	CB-CA-C	-10.89	97.43	112.14
13	s	342	ASN	N-CA-C	-10.77	87.87	110.80
9	a	500	VAL	CB-CA-C	10.68	122.52	110.88
1	C	196	PHE	CB-CA-C	-10.52	93.03	109.34
15	q	51	MET	N-CA-C	10.49	125.28	113.21
1	B	136	THR	O-C-N	-10.40	113.43	121.55
1	A	463	GLU	CA-C-N	10.38	135.23	120.28
1	A	463	GLU	C-N-CA	10.38	135.23	120.28
6	L	98	TYR	N-CA-C	10.35	124.80	109.07
2	E	391	PRO	N-CA-C	-10.24	91.37	112.47
1	A	535	TYR	CA-C-N	-10.24	105.53	120.28
1	A	535	TYR	C-N-CA	-10.24	105.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	370	TYR	CB-CA-C	-10.13	90.25	110.42
7	M	111	HIS	CB-CA-C	10.08	130.02	110.17
13	s	348	ASN	N-CA-C	-9.94	89.63	110.80
6	L	104	SER	N-CA-C	-9.88	100.50	111.07
13	s	421	SER	CA-C-N	-9.80	109.74	119.64
13	s	421	SER	C-N-CA	-9.80	109.74	119.64
1	A	526	THR	CA-C-N	9.78	132.06	119.84
1	A	526	THR	C-N-CA	9.78	132.06	119.84
10	b	44	THR	N-CA-C	9.63	121.72	111.03
8	P	83	HIS	N-CA-C	9.61	124.62	113.19
7	N	112	PRO	N-CA-C	9.59	132.23	112.47
1	B	592	ASP	N-CA-CB	9.56	126.66	110.49
2	E	164	ILE	CA-C-N	9.55	139.09	120.94
2	E	164	ILE	C-N-CA	9.55	139.09	120.94
7	O	110	VAL	N-CA-C	-9.26	90.09	109.34
5	I	161	ARG	N-CA-C	-9.16	91.28	110.80
2	F	164	ILE	CA-C-N	9.15	133.10	120.65
2	F	164	ILE	C-N-CA	9.15	133.10	120.65
1	B	17	THR	N-CA-C	9.05	130.07	110.80
1	A	535	TYR	N-CA-C	-8.99	101.39	111.82
7	O	107	ARG	CA-C-N	8.98	128.92	119.85
7	O	107	ARG	C-N-CA	8.98	128.92	119.85
7	M	112	PRO	CA-C-N	8.94	137.79	121.70
7	M	112	PRO	C-N-CA	8.94	137.79	121.70
1	C	18	PHE	CA-C-N	8.93	132.49	122.67
1	C	18	PHE	C-N-CA	8.93	132.49	122.67
2	D	147	ALA	N-CA-C	8.88	124.25	111.56
9	a	6	ARG	N-CA-C	8.88	124.82	112.04
13	s	305	ALA	O-C-N	-8.82	112.49	123.17
1	B	592	ASP	CA-C-N	8.77	138.61	121.41
1	B	592	ASP	C-N-CA	8.77	138.61	121.41
13	s	421	SER	N-CA-C	-8.76	90.46	109.81
2	E	389	TYR	C-N-CD	-8.63	89.60	125.00
1	C	196	PHE	N-CA-C	8.52	124.29	113.55
9	a	493	GLU	N-CA-C	-8.46	102.06	111.28
9	a	223	PHE	N-CA-C	8.38	120.11	110.97
1	A	139	LYS	CA-C-N	8.31	137.41	121.54
1	A	139	LYS	C-N-CA	8.31	137.41	121.54
9	a	517	PHE	O-C-N	-8.18	111.94	123.06
7	N	112	PRO	CA-C-N	8.14	136.35	121.70
7	N	112	PRO	C-N-CA	8.14	136.35	121.70
1	A	535	TYR	CE1-CZ-OH	-8.09	95.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	332	SER	N-CA-C	-7.96	99.61	110.68
9	a	6	ARG	CB-CA-C	-7.96	96.00	110.56
1	B	122	VAL	N-CA-C	7.84	118.79	106.88
1	B	351	THR	N-CA-C	-7.83	102.81	113.30
13	s	265	ILE	N-CA-C	7.82	119.54	109.30
1	C	198	GLY	CA-C-N	7.79	132.40	121.96
1	C	198	GLY	C-N-CA	7.79	132.40	121.96
12	e	70	ASN	N-CA-C	7.78	127.36	110.80
11	d	346	ASN	N-CA-C	-7.75	95.07	108.56
1	B	592	ASP	CB-CA-C	-7.73	95.04	110.42
5	K	164	ASP	N-CA-C	-7.70	97.90	109.83
1	C	17	THR	CB-CA-C	-7.69	95.45	109.15
5	J	165	VAL	CB-CA-C	7.67	123.87	111.29
1	C	458	MET	N-CA-C	-7.64	101.88	112.12
1	B	558	THR	N-CA-C	7.62	121.04	112.97
7	O	112	PRO	CA-C-O	-7.58	106.80	120.60
13	s	342	ASN	CA-C-N	7.51	134.74	121.75
13	s	342	ASN	C-N-CA	7.51	134.74	121.75
1	B	588	ASP	N-CA-C	7.49	126.37	109.81
2	F	147	ALA	N-CA-C	7.49	121.39	111.28
12	e	78	PHE	CA-C-N	7.47	135.81	121.54
12	e	78	PHE	C-N-CA	7.47	135.81	121.54
6	L	101	ALA	N-CA-C	7.43	126.62	110.80
6	L	106	LEU	N-CA-C	7.37	121.14	108.02
6	L	105	ILE	CA-C-N	-7.28	112.52	122.86
6	L	105	ILE	C-N-CA	-7.28	112.52	122.86
2	F	89	VAL	CB-CA-C	-7.27	99.79	110.62
8	P	443	VAL	CB-CA-C	7.25	122.22	112.22
11	d	157	ASP	N-CA-C	7.25	121.54	113.21
14	r	325	THR	O-C-N	7.20	129.87	122.09
8	P	293	GLN	N-CA-C	7.20	120.99	112.93
2	D	89	VAL	CB-CA-C	-7.18	99.84	110.33
13	s	305	ALA	CA-C-N	7.16	134.14	121.75
13	s	305	ALA	C-N-CA	7.16	134.14	121.75
3	G	326	LYS	CB-CA-C	-7.13	99.74	111.36
2	D	212	LEU	CA-C-N	7.12	135.32	122.43
2	D	212	LEU	C-N-CA	7.12	135.32	122.43
1	A	535	TYR	O-C-N	7.09	130.99	122.27
8	P	336	GLU	N-CA-C	-7.08	103.56	111.28
4	H	75	THR	CB-CA-C	7.06	122.86	110.85
4	H	123	GLY	N-CA-C	-7.04	98.97	110.95
2	D	212	LEU	CB-CA-C	-7.04	98.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	103	ASP	CB-CA-C	7.02	122.65	110.01
4	H	11	PRO	CB-CA-C	-7.00	105.03	111.40
8	P	289	LEU	N-CA-C	-6.96	103.62	111.07
1	A	526	THR	N-CA-CB	-6.95	99.69	110.11
12	e	72	THR	CA-C-O	-6.91	113.22	120.55
1	C	456	LYS	CD-CE-NZ	-6.88	89.87	111.90
1	B	349	ASP	N-CA-C	6.82	120.44	107.75
7	M	108	PRO	N-CA-C	6.74	126.36	112.47
2	D	249	GLU	N-CA-CB	-6.72	100.27	110.01
9	a	194	ASN	N-CA-C	6.69	120.64	111.54
7	M	111	HIS	N-CA-C	-6.66	95.10	109.81
6	L	106	LEU	CA-C-O	-6.60	113.20	120.33
8	P	70	GLY	N-CA-C	-6.58	97.60	113.18
1	A	463	GLU	N-CA-C	6.56	119.02	111.02
1	C	198	GLY	N-CA-C	-6.54	97.69	113.18
15	o	51	MET	N-CA-C	6.54	120.73	113.21
6	L	11	ILE	CB-CA-C	-6.48	104.15	111.80
2	E	211	GLY	N-CA-C	6.46	123.24	110.77
10	b	22	VAL	O-C-N	-6.43	114.53	121.80
7	M	113	ASN	N-CA-CB	-6.42	99.58	110.50
7	N	111	HIS	CA-C-N	-6.41	111.83	119.84
7	N	111	HIS	C-N-CA	-6.41	111.83	119.84
14	r	329	ILE	CB-CA-C	-6.38	101.51	110.95
1	C	199	ILE	CB-CA-C	6.36	120.64	111.80
2	E	289	CYS	CB-CA-C	6.36	120.23	110.62
2	E	289	CYS	N-CA-C	-6.34	96.73	108.02
1	B	472	PHE	CA-C-N	6.34	124.23	120.24
1	B	472	PHE	C-N-CA	6.34	124.23	120.24
11	d	230	THR	CB-CA-C	-6.34	98.67	109.51
8	P	289	LEU	CB-CA-C	6.32	120.80	110.88
5	K	157	VAL	CB-CA-C	6.32	120.94	112.22
1	C	143	VAL	CA-C-N	-6.27	109.77	121.93
1	C	143	VAL	C-N-CA	-6.27	109.77	121.93
9	a	84	GLU	CB-CA-C	6.23	119.06	110.34
8	P	333	SER	CA-C-N	6.22	133.41	121.54
8	P	333	SER	C-N-CA	6.22	133.41	121.54
6	L	95	GLU	CA-C-N	6.20	136.92	121.80
6	L	95	GLU	C-N-CA	6.20	136.92	121.80
12	e	25	PRO	CA-C-N	-6.15	111.27	121.92
12	e	25	PRO	C-N-CA	-6.15	111.27	121.92
1	B	268	ASN	N-CA-C	6.15	123.90	110.80
9	a	479	TRP	N-CA-C	-6.14	104.86	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	THR	CA-C-N	6.14	127.52	119.84
1	B	136	THR	C-N-CA	6.14	127.52	119.84
1	A	534	PHE	CA-C-N	6.09	129.57	120.31
1	A	534	PHE	C-N-CA	6.09	129.57	120.31
2	D	213	VAL	N-CA-C	-6.09	99.50	109.12
9	a	769	SER	N-CA-C	6.09	120.78	112.68
1	A	468	HIS	N-CA-C	6.08	122.16	114.31
6	L	98	TYR	N-CA-CB	-6.08	101.50	111.66
7	M	109	GLN	CA-C-N	-6.08	114.33	123.27
7	M	109	GLN	C-N-CA	-6.08	114.33	123.27
12	e	58	ALA	N-CA-C	-6.08	103.98	112.25
8	P	331	LEU	O-C-N	6.06	129.35	122.20
9	a	329	ASP	N-CA-C	6.03	120.15	113.21
1	A	462	ASP	CA-C-N	-6.02	112.42	120.79
1	A	462	ASP	C-N-CA	-6.02	112.42	120.79
9	a	821	PHE	CB-CA-C	5.98	120.62	109.86
13	s	264	ARG	CA-C-N	5.94	129.36	120.69
13	s	264	ARG	C-N-CA	5.94	129.36	120.69
4	H	129	GLU	N-CA-C	-5.93	106.69	114.04
1	A	535	TYR	OH-CZ-CE2	5.91	137.64	119.90
2	E	393	ASN	O-C-N	-5.90	114.45	122.48
12	e	70	ASN	CB-CA-C	-5.90	98.67	110.42
7	O	45	ASP	CB-CA-C	5.87	122.36	110.38
9	a	498	ASN	CA-C-N	5.86	127.17	119.84
9	a	498	ASN	C-N-CA	5.86	127.17	119.84
1	B	17	THR	CB-CA-C	-5.85	98.79	110.42
2	E	388	ILE	CA-C-N	-5.84	112.57	121.92
2	E	388	ILE	C-N-CA	-5.84	112.57	121.92
5	K	154	VAL	CB-CA-C	-5.83	104.38	112.02
9	a	10	MET	CB-CA-C	-5.81	99.25	109.71
9	a	84	GLU	N-CA-C	-5.80	98.36	107.93
9	a	495	LEU	N-CA-C	5.80	117.60	111.28
6	L	98	TYR	CA-C-N	5.79	132.60	121.54
6	L	98	TYR	C-N-CA	5.79	132.60	121.54
1	A	473	VAL	CB-CA-C	-5.74	108.25	113.70
15	p	51	MET	N-CA-C	5.72	117.86	110.65
2	E	390	PRO	N-CA-C	-5.72	103.73	110.70
5	K	162	ASP	CB-CA-C	-5.70	101.00	114.16
1	C	297	GLU	N-CA-C	5.69	118.07	107.99
11	d	91	GLU	CA-C-N	-5.68	112.74	119.84
11	d	91	GLU	C-N-CA	-5.68	112.74	119.84
1	A	532	CYS	CA-C-N	5.67	126.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	CYS	C-N-CA	5.67	126.93	119.84
3	G	180	GLU	CB-CA-C	5.65	120.23	110.84
4	H	11	PRO	N-CA-C	5.65	119.48	110.21
1	C	268	ASN	N-CA-C	5.64	119.86	113.15
9	a	222	ILE	N-CA-C	-5.64	97.61	109.34
7	N	113	ASN	N-CA-CB	-5.60	100.98	110.50
9	a	482	ARG	CA-C-N	5.60	126.84	119.84
9	a	482	ARG	C-N-CA	5.60	126.84	119.84
1	B	266	TYR	CB-CA-C	5.59	121.55	110.42
9	a	193	GLY	CA-C-N	5.59	130.06	122.07
9	a	193	GLY	C-N-CA	5.59	130.06	122.07
8	P	68	THR	N-CA-C	5.55	122.63	110.80
9	a	228	GLN	N-CA-C	-5.51	106.49	113.43
8	P	346	LEU	N-CA-C	5.49	118.76	111.30
1	C	297	GLU	CB-CA-C	-5.48	101.86	110.79
11	d	61	GLU	N-CA-C	5.47	118.08	111.40
13	s	363	SER	N-CA-C	5.46	122.44	110.80
1	B	349	ASP	CA-C-N	5.45	131.96	121.54
1	B	349	ASP	C-N-CA	5.45	131.96	121.54
2	F	464	ALA	N-CA-C	5.45	117.60	108.23
10	b	15	PHE	O-C-N	-5.44	116.15	122.03
10	b	15	PHE	CB-CA-C	-5.42	102.55	110.95
1	B	346	MET	O-C-N	-5.38	117.19	123.27
1	B	138	CYS	CA-C-N	5.37	131.80	121.54
1	B	138	CYS	C-N-CA	5.37	131.80	121.54
13	s	362	PRO	CB-CA-C	-5.37	102.69	111.56
13	s	307	LEU	CA-C-N	-5.37	116.53	123.19
13	s	307	LEU	C-N-CA	-5.37	116.53	123.19
7	M	108	PRO	CB-CA-C	-5.37	102.71	111.56
9	a	223	PHE	CA-C-N	5.36	131.78	121.54
9	a	223	PHE	C-N-CA	5.36	131.78	121.54
5	K	152	ILE	CB-CA-C	-5.36	101.61	111.36
7	N	111	HIS	CA-CB-CG	-5.36	108.44	113.80
9	a	47	PHE	CA-C-N	5.34	130.14	122.40
9	a	47	PHE	C-N-CA	5.34	130.14	122.40
6	L	95	GLU	N-CA-C	-5.34	99.71	108.41
9	a	528	ASN	N-CA-C	5.33	119.34	113.21
10	b	16	TRP	CA-C-N	-5.32	113.10	120.38
10	b	16	TRP	C-N-CA	-5.32	113.10	120.38
13	s	270	GLN	N-CA-C	-5.31	99.49	110.80
9	a	311	ASN	N-CA-C	5.31	117.14	110.24
9	a	501	LEU	CA-CB-CG	5.30	134.84	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	44	THR	CB-CA-C	-5.28	102.77	110.95
2	E	393	ASN	CA-C-N	5.27	129.57	121.19
2	E	393	ASN	C-N-CA	5.27	129.57	121.19
11	d	281	ALA	N-CA-C	5.26	118.38	111.28
3	G	178	ASP	CA-C-N	5.25	131.56	121.54
3	G	178	ASP	C-N-CA	5.25	131.56	121.54
2	E	90	SER	N-CA-C	-5.24	99.12	108.13
9	a	310	CYS	CA-C-N	5.22	128.50	120.82
9	a	310	CYS	C-N-CA	5.22	128.50	120.82
7	M	113	ASN	CA-C-O	5.21	129.66	120.80
1	A	467	LYS	N-CA-C	-5.21	107.09	113.50
7	N	112	PRO	CA-C-O	-5.20	111.13	120.60
2	E	489	LYS	CA-C-N	5.19	129.71	122.08
2	E	489	LYS	C-N-CA	5.19	129.71	122.08
1	A	533	PRO	CB-CA-C	-5.18	103.00	111.56
9	a	821	PHE	N-CA-C	-5.18	100.16	108.55
2	E	90	SER	CB-CA-C	5.16	117.77	110.24
7	N	56	GLN	N-CA-C	-5.16	107.64	114.04
8	P	443	VAL	N-CA-C	-5.14	105.53	110.72
13	s	448	LEU	CA-CB-CG	5.09	134.13	116.30
13	s	265	ILE	CB-CA-C	-5.09	103.67	111.71
7	M	68	ASN	O-C-N	-5.09	115.44	122.46
13	s	375	GLU	CA-CB-CG	5.08	124.26	114.10
8	P	105	HIS	CA-C-N	5.08	129.49	121.56
8	P	105	HIS	C-N-CA	5.08	129.49	121.56
9	a	769	SER	CB-CA-C	-5.07	101.77	110.24
13	s	343	LEU	N-CA-C	-5.07	101.36	109.07
9	a	312	ILE	CA-C-N	5.07	131.01	123.05
9	a	312	ILE	C-N-CA	5.07	131.01	123.05
5	J	165	VAL	N-CA-C	-5.06	98.82	109.34
5	J	164	ASP	N-CA-C	-5.04	104.46	110.41
1	A	268	ASN	N-CA-C	5.04	119.01	113.21
16	f	17	VAL	N-CA-C	-5.03	106.54	111.77
9	a	500	VAL	CA-C-N	5.02	131.13	121.54
9	a	500	VAL	C-N-CA	5.02	131.13	121.54
8	P	67	GLN	CA-C-N	5.01	131.11	121.54
8	P	67	GLN	C-N-CA	5.01	131.11	121.54
1	B	122	VAL	CB-CA-C	-5.01	104.95	111.81

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	ASP	Mainchain
1	A	533	PRO	Mainchain
1	A	535	TYR	Sidechain
1	B	591	LYS	Mainchain
1	C	455	SER	Mainchain
2	D	249	GLU	Mainchain
5	I	161	ARG	Mainchain
7	M	110	VAL	Mainchain
7	N	110	VAL	Mainchain
8	P	369	ASN	Peptide
9	a	480	SER	Mainchain
13	s	366	SER	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4568	0	4550	79	0
1	B	4582	0	4565	88	0
1	C	4628	0	4611	58	0
2	D	3609	0	3611	68	0
2	E	3585	0	3580	54	0
2	F	3594	0	3593	40	0
3	G	2823	0	2876	34	0
4	H	1700	0	1812	53	0
5	I	1614	0	1563	17	0
5	J	1624	0	1592	33	0
5	K	1595	0	1527	22	0
6	L	816	0	815	26	0
7	M	665	0	507	13	0
7	N	665	0	507	5	0
7	O	665	0	507	11	0
8	P	2819	0	2647	48	0
9	a	6093	0	6131	212	0
10	b	1503	0	1549	40	0
11	d	2819	0	2756	46	0
12	e	590	0	613	76	0
13	s	1668	0	1554	99	0
14	r	385	0	373	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	c	1064	0	1132	10	0
15	g	1064	0	1132	8	0
15	k	1064	0	1132	11	0
15	l	1064	0	1132	11	0
15	m	1064	0	1132	13	0
15	n	1064	0	1132	17	0
15	o	1073	0	1145	12	0
15	p	1073	0	1145	11	0
15	q	1073	0	1145	16	0
16	f	351	0	358	6	0
17	C	1	0	0	0	0
18	C	27	0	12	1	0
19	b	213	0	286	16	0
19	g	43	0	59	6	0
19	p	44	0	60	1	0
19	r	94	0	132	3	0
20	s	84	0	78	11	0
21	r	20	0	33	1	0
All	All	63090	0	63084	1101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASP:HB3	1:B:589:PRO:CD	1.19	1.54
9:a:481:VAL:CG1	9:a:510:VAL:CG1	1.80	1.54
9:a:481:VAL:CG1	9:a:510:VAL:HG13	1.05	1.49
9:a:481:VAL:HG11	9:a:510:VAL:CA	1.39	1.47
9:a:496:ARG:CZ	12:e:70:ASN:HD22	1.29	1.44
13:s:404:ASN:ND2	20:s:506:NAG:C3	1.81	1.44
9:a:481:VAL:HG12	9:a:510:VAL:CG1	1.44	1.40
1:B:588:ASP:CB	1:B:589:PRO:HD2	1.30	1.37
9:a:496:ARG:NH2	12:e:70:ASN:HD22	0.88	1.37
9:a:496:ARG:NH2	12:e:70:ASN:ND2	1.67	1.32
4:H:75:THR:HG21	4:H:130:GLN:NE2	1.42	1.31
2:E:389:TYR:CD2	2:E:390:PRO:HD3	1.66	1.30
9:a:496:ARG:CZ	12:e:70:ASN:ND2	1.85	1.29
9:a:481:VAL:HG11	9:a:510:VAL:CB	1.62	1.27
1:C:196:PHE:CD1	1:C:196:PHE:O	1.91	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:281:GLU:HG2	13:s:315:PHE:CZ	1.74	1.22
9:a:483:PRO:HG2	12:e:80:TRP:CZ2	1.74	1.20
7:O:111:HIS:CD2	7:O:112:PRO:HD2	1.77	1.19
9:a:482:ARG:CB	9:a:483:PRO:HD3	1.65	1.19
13:s:345:ILE:HD11	13:s:393:MET:HE3	1.24	1.16
9:a:480:SER:CB	9:a:522:ILE:HD13	1.74	1.16
9:a:480:SER:HB3	9:a:522:ILE:HD13	1.31	1.13
9:a:482:ARG:HB2	9:a:483:PRO:CD	1.67	1.12
13:s:283:LEU:HD21	13:s:314:LEU:HD21	1.28	1.10
2:E:389:TYR:CD2	2:E:390:PRO:CD	2.34	1.09
9:a:481:VAL:CG1	9:a:510:VAL:HA	1.82	1.08
9:a:481:VAL:HG13	9:a:510:VAL:HG13	1.35	1.08
13:s:268:TRP:CH2	13:s:270:GLN:NE2	2.21	1.08
8:P:370:TYR:O	8:P:374:LYS:HG3	1.55	1.07
13:s:281:GLU:CG	13:s:315:PHE:CZ	2.36	1.07
9:a:481:VAL:HG11	9:a:510:VAL:HA	1.10	1.07
9:a:481:VAL:CG1	9:a:510:VAL:CA	2.35	1.05
1:A:532:CYS:SG	1:A:536:LYS:HD3	1.96	1.04
9:a:481:VAL:HG11	9:a:510:VAL:CG1	1.67	1.03
13:s:347:SER:HB3	13:s:391:TRP:CZ2	1.93	1.03
9:a:528:ASN:ND2	12:e:67:GLN:HB2	1.73	1.01
1:B:263:LEU:HA	1:B:267:SER:HB3	1.40	1.01
13:s:404:ASN:HD22	20:s:506:NAG:C3	1.72	1.00
2:D:287:TYR:HB2	2:D:344:ARG:HD3	1.43	0.99
1:B:535:TYR:OH	1:B:592:ASP:OD1	1.81	0.99
1:B:263:LEU:O	1:B:267:SER:OG	1.81	0.98
9:a:496:ARG:NE	12:e:70:ASN:ND2	2.12	0.98
1:B:266:TYR:HB2	1:B:531:PHE:CE1	1.99	0.98
13:s:286:ARG:O	13:s:290:VAL:HG11	1.62	0.98
7:O:111:HIS:HD2	7:O:112:PRO:HD2	1.07	0.97
12:e:23:ALA:O	12:e:27:PHE:HD1	1.48	0.97
11:d:137:GLN:O	11:d:138:MET:HG2	1.64	0.96
13:s:274:VAL:HG21	13:s:321:PHE:CZ	1.99	0.96
6:L:69:TYR:HB2	6:L:96:HIS:HD2	1.28	0.96
9:a:507:VAL:HG11	9:a:601:LYS:CA	1.96	0.95
1:A:535:TYR:HA	1:A:538:VAL:HG22	1.48	0.95
9:a:528:ASN:CG	12:e:67:GLN:HB2	1.89	0.95
4:H:75:THR:HG21	4:H:130:GLN:HE21	1.23	0.95
1:B:263:LEU:HA	1:B:267:SER:CB	1.98	0.94
9:a:483:PRO:HG2	12:e:80:TRP:HZ2	1.23	0.94
2:E:389:TYR:CG	2:E:390:PRO:HD3	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:389:TYR:CG	2:E:390:PRO:CD	2.51	0.94
8:P:284:ARG:NH1	8:P:287:TYR:HE2	1.66	0.94
6:L:99:ASP:OD1	6:L:99:ASP:C	2.10	0.93
13:s:347:SER:HB3	13:s:391:TRP:HZ2	1.33	0.93
6:L:69:TYR:HB2	6:L:96:HIS:CD2	2.03	0.92
9:a:496:ARG:HH21	12:e:70:ASN:HD22	0.96	0.92
1:A:532:CYS:SG	1:A:536:LYS:HB3	2.09	0.91
9:a:480:SER:HB2	9:a:522:ILE:HD13	1.49	0.91
1:B:17:THR:HG22	1:B:18:PHE:CD1	2.06	0.91
2:D:249:GLU:CA	2:D:254:MET:HE2	2.00	0.91
9:a:503:LEU:CD1	9:a:528:ASN:HD21	1.85	0.90
1:B:528:TYR:HB3	1:B:588:ASP:OD1	1.70	0.90
13:s:404:ASN:HD21	20:s:506:NAG:C3	1.66	0.90
1:B:260:SER:O	1:B:263:LEU:HG	1.70	0.90
5:I:155:TYR:CE1	5:I:163:VAL:HG12	2.06	0.90
4:H:75:THR:CG2	4:H:130:GLN:NE2	2.34	0.90
1:B:17:THR:HG22	1:B:18:PHE:CE1	2.08	0.89
2:E:389:TYR:CE2	2:E:390:PRO:HD3	2.08	0.89
5:I:155:TYR:CE1	5:I:163:VAL:CG1	2.56	0.88
9:a:526:ALA:HA	12:e:68:LEU:HD23	1.55	0.88
2:E:390:PRO:O	2:E:392:ILE:N	2.06	0.88
13:s:287:THR:OG1	13:s:311:TYR:OH	1.87	0.88
9:a:495:LEU:CD2	12:e:74:TRP:HD1	1.87	0.87
5:J:152:ILE:N	5:J:153:PRO:HD2	1.88	0.87
13:s:283:LEU:HD21	13:s:314:LEU:CD2	2.04	0.87
13:s:345:ILE:HD11	13:s:393:MET:CE	2.03	0.86
9:a:481:VAL:CG1	9:a:510:VAL:CB	2.32	0.86
1:C:196:PHE:O	1:C:196:PHE:HD1	1.49	0.86
8:P:329:GLN:HA	8:P:332:SER:HB3	1.59	0.85
13:s:283:LEU:CD2	13:s:314:LEU:HD21	2.06	0.85
5:I:155:TYR:CD1	5:I:163:VAL:CG1	2.59	0.84
8:P:284:ARG:NH1	8:P:287:TYR:CE2	2.45	0.84
4:H:75:THR:CG2	4:H:130:GLN:HE21	1.89	0.84
13:s:404:ASN:ND2	20:s:506:NAG:C4	2.41	0.84
3:G:119:LYS:O	3:G:123:GLU:HG2	1.78	0.84
4:H:69:LEU:CD1	4:H:134:LEU:HD21	2.07	0.84
19:b:301:POV:O13	13:s:333:SER:CB	2.27	0.83
5:K:163:VAL:HB	5:K:165:VAL:HG23	1.61	0.82
13:s:268:TRP:HH2	13:s:270:GLN:HE22	1.24	0.82
5:K:162:ASP:OD1	5:K:162:ASP:N	2.12	0.82
9:a:481:VAL:HG21	9:a:510:VAL:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:347:SER:CB	13:s:391:TRP:HZ2	1.93	0.82
8:P:286:GLU:O	8:P:290:ALA:HB3	1.80	0.81
8:P:279:VAL:O	8:P:280:GLU:HG3	1.80	0.81
8:P:284:ARG:HD3	8:P:287:TYR:CE2	2.14	0.81
1:C:196:PHE:CD1	1:C:196:PHE:C	2.54	0.81
9:a:527:THR:N	12:e:67:GLN:O	2.14	0.81
1:B:528:TYR:CB	1:B:588:ASP:OD1	2.29	0.80
1:B:588:ASP:HB2	1:B:590:VAL:HG12	1.64	0.80
1:C:76:GLY:O	7:M:113:ASN:ND2	2.16	0.79
1:A:534:PHE:CE1	1:A:537:THR:HB	2.17	0.79
9:a:495:LEU:HD21	12:e:74:TRP:HD1	1.47	0.79
5:J:153:PRO:O	5:J:157:VAL:HG23	1.83	0.79
8:P:284:ARG:HH11	8:P:287:TYR:HE2	1.22	0.79
13:s:348:ASN:O	13:s:350:SER:N	2.15	0.79
9:a:528:ASN:O	9:a:531:THR:HG22	1.83	0.78
9:a:507:VAL:HG11	9:a:601:LYS:N	1.98	0.78
13:s:354:PHE:HZ	13:s:391:TRP:O	1.67	0.78
13:s:281:GLU:HG3	13:s:315:PHE:CZ	2.17	0.78
9:a:503:LEU:CD1	9:a:528:ASN:ND2	2.47	0.78
1:C:17:THR:O	1:C:17:THR:HG22	1.82	0.77
19:b:301:POV:O13	13:s:333:SER:HB2	1.83	0.77
13:s:286:ARG:O	13:s:290:VAL:CG1	2.32	0.77
2:D:249:GLU:HB2	2:D:254:MET:CE	2.15	0.76
1:A:472:PHE:CD1	1:A:538:VAL:HG12	2.20	0.76
8:P:278:SER:OG	8:P:283:THR:HG22	1.86	0.76
2:E:389:TYR:CB	2:E:390:PRO:HD2	2.15	0.76
5:J:151:ALA:C	5:J:153:PRO:HD2	2.11	0.76
10:b:16:TRP:O	10:b:17:ALA:C	2.25	0.76
12:e:24:GLY:O	12:e:28:VAL:HG23	1.85	0.76
2:D:249:GLU:HA	2:D:254:MET:HE2	1.67	0.75
9:a:528:ASN:CG	12:e:67:GLN:CB	2.58	0.75
8:P:278:SER:OG	8:P:283:THR:CG2	2.34	0.74
9:a:496:ARG:NH2	12:e:70:ASN:CG	2.45	0.74
9:a:596:THR:O	12:e:61:ASN:ND2	2.20	0.74
10:b:38:ALA:O	10:b:42:THR:OG1	2.04	0.74
2:E:389:TYR:CD2	2:E:390:PRO:HD2	2.23	0.74
1:A:532:CYS:SG	1:A:536:LYS:CD	2.74	0.73
9:a:528:ASN:OD1	12:e:67:GLN:N	2.17	0.73
9:a:482:ARG:H	9:a:482:ARG:HD2	1.54	0.72
13:s:404:ASN:ND2	20:s:506:NAG:O4	2.22	0.72
9:a:495:LEU:O	12:e:70:ASN:OD1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:152:ILE:N	5:J:153:PRO:CD	2.52	0.72
4:H:77:GLY:O	4:H:78:ASP:OD1	2.08	0.72
9:a:480:SER:CB	9:a:522:ILE:CD1	2.63	0.71
9:a:481:VAL:CG2	9:a:510:VAL:HA	2.19	0.71
9:a:482:ARG:HG3	9:a:482:ARG:HH11	1.56	0.71
11:d:331:TRP:NE1	11:d:346:ASN:O	2.23	0.71
9:a:496:ARG:CZ	12:e:70:ASN:HD21	2.01	0.71
12:e:23:ALA:O	12:e:27:PHE:CD1	2.38	0.71
19:b:301:POV:O13	13:s:333:SER:HB3	1.90	0.71
9:a:481:VAL:HG12	9:a:510:VAL:HG12	1.68	0.71
9:a:496:ARG:NE	12:e:70:ASN:HD21	1.86	0.71
13:s:281:GLU:HG3	13:s:315:PHE:CE2	2.26	0.71
9:a:482:ARG:HA	9:a:482:ARG:NE	2.04	0.70
9:a:483:PRO:CG	12:e:80:TRP:CZ2	2.66	0.70
9:a:525:ILE:HG23	12:e:68:LEU:CD2	2.21	0.70
15:p:51:MET:O	15:p:55:SER:OG	2.04	0.70
1:A:459:ARG:HD3	1:A:459:ARG:N	2.06	0.70
9:a:479:TRP:HB3	9:a:522:ILE:HG21	1.73	0.70
5:I:155:TYR:CD1	5:I:163:VAL:HG13	2.25	0.70
4:H:156:VAL:HG23	6:L:105:ILE:HD13	1.74	0.70
9:a:363:THR:HG22	9:a:821:PHE:O	1.92	0.70
9:a:481:VAL:HG11	9:a:510:VAL:C	2.14	0.70
9:a:483:PRO:CG	12:e:80:TRP:HZ2	2.03	0.70
1:A:472:PHE:HD1	1:A:538:VAL:HG12	1.55	0.69
9:a:495:LEU:HD21	12:e:74:TRP:CD1	2.26	0.69
9:a:480:SER:HB2	9:a:522:ILE:CD1	2.20	0.69
9:a:507:VAL:HG11	9:a:601:LYS:CB	2.22	0.69
9:a:498:ASN:HB3	9:a:499:PRO:HD3	1.73	0.69
9:a:507:VAL:HG11	9:a:601:LYS:HB2	1.74	0.69
13:s:332:VAL:HA	15:g:9:GLU:HB2	1.75	0.69
6:L:90:GLU:OE1	6:L:101:ALA:HB3	1.91	0.69
9:a:500:VAL:O	12:e:70:ASN:N	2.25	0.69
2:E:389:TYR:CG	2:E:390:PRO:HD2	2.27	0.69
4:H:193:GLU:HG2	4:H:196:ARG:HH21	1.58	0.69
7:M:110:VAL:O	7:M:111:HIS:C	2.32	0.69
13:s:281:GLU:HG2	13:s:315:PHE:HZ	1.53	0.69
1:A:266:TYR:CD1	1:A:531:PHE:HB2	2.28	0.68
2:D:249:GLU:HG3	5:J:77:ASN:ND2	2.07	0.68
2:D:249:GLU:HG3	5:J:77:ASN:HD22	1.57	0.68
8:P:284:ARG:HD3	8:P:287:TYR:CD2	2.27	0.68
9:a:496:ARG:NH2	12:e:70:ASN:CB	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:332:VAL:HG11	15:c:10:TYR:OH	1.94	0.68
1:B:588:ASP:HB3	1:B:589:PRO:HD3	1.63	0.68
13:s:270:GLN:HE21	13:s:270:GLN:CA	2.07	0.68
8:P:370:TYR:O	8:P:374:LYS:CG	2.36	0.68
9:a:481:VAL:HG12	9:a:510:VAL:HG13	0.68	0.68
10:b:39:TRP:HH2	13:s:420:PHE:O	1.77	0.68
13:s:404:ASN:HD21	20:s:506:NAG:C4	2.04	0.67
1:B:263:LEU:HA	1:B:267:SER:OG	1.94	0.67
9:a:482:ARG:HB3	9:a:482:ARG:NH1	2.10	0.67
9:a:482:ARG:HH11	9:a:482:ARG:CG	2.08	0.67
9:a:495:LEU:CD2	12:e:74:TRP:CD1	2.75	0.66
12:e:24:GLY:O	12:e:28:VAL:CG2	2.44	0.66
3:G:264:GLU:HA	3:G:267:ARG:HB2	1.76	0.66
5:K:152:ILE:N	5:K:153:PRO:HD2	2.10	0.66
5:K:152:ILE:HB	5:K:153:PRO:HD3	1.77	0.66
1:B:266:TYR:HB2	1:B:531:PHE:HE1	1.55	0.66
9:a:434:LYS:O	9:a:435:ASN:OD1	2.14	0.66
9:a:507:VAL:HG11	9:a:601:LYS:HA	1.76	0.65
13:s:281:GLU:HG2	13:s:315:PHE:CE1	2.29	0.65
9:a:507:VAL:CG1	9:a:601:LYS:HB2	2.27	0.65
1:B:263:LEU:C	1:B:267:SER:OG	2.39	0.65
2:D:249:GLU:CB	2:D:254:MET:HE2	2.26	0.65
1:B:588:ASP:CB	1:B:589:PRO:CD	2.04	0.65
10:b:34:ARG:HH21	19:b:304:POV:H14	1.61	0.65
6:L:99:ASP:OD1	6:L:100:ALA:N	2.29	0.65
10:b:35:PHE:HB3	19:b:301:POV:H34	1.78	0.65
7:O:110:VAL:HG12	7:O:111:HIS:H	1.62	0.65
9:a:496:ARG:NH2	12:e:70:ASN:HB3	2.11	0.65
1:C:387:GLU:HG3	2:E:264:ALA:HB3	1.79	0.64
9:a:461:GLY:O	9:a:465:ASN:O	2.15	0.64
9:a:482:ARG:HD2	9:a:482:ARG:N	2.10	0.64
15:c:72:VAL:HG21	15:c:99:VAL:HG11	1.78	0.64
4:H:40:LEU:HD23	4:H:162:ILE:CG1	2.27	0.64
2:D:249:GLU:HB2	2:D:254:MET:HE2	1.78	0.64
3:G:326:LYS:O	3:G:326:LYS:HG3	1.97	0.64
4:H:152:GLN:OE1	6:L:102:LYS:NZ	2.31	0.63
1:C:17:THR:O	1:C:17:THR:CG2	2.46	0.63
9:a:522:ILE:HG13	12:e:66:PRO:HG3	1.80	0.63
12:e:55:ALA:O	12:e:59:GLN:HG3	1.98	0.63
2:D:208:ARG:HD2	2:D:251:ASN:CG	2.24	0.63
4:H:40:LEU:HB3	4:H:162:ILE:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:LYS:O	2:D:249:GLU:HB3	1.99	0.63
1:B:590:VAL:HG22	1:B:590:VAL:O	1.99	0.63
5:K:152:ILE:O	5:K:152:ILE:HG22	1.98	0.63
1:C:588:ASP:HB3	1:C:590:VAL:HG22	1.81	0.62
9:a:485:PHE:O	9:a:489:ASN:HB2	1.98	0.62
15:m:72:VAL:HG21	15:m:99:VAL:HG11	1.79	0.62
6:L:91:ILE:HB	6:L:92:PRO:HD2	1.81	0.62
9:a:6:ARG:O	9:a:7:SER:HB2	1.98	0.62
10:b:19:LEU:HD13	10:b:19:LEU:O	1.98	0.62
11:d:121:SER:HB3	11:d:145:GLN:HG2	1.82	0.62
9:a:481:VAL:HG13	9:a:510:VAL:HG22	1.82	0.62
1:A:535:TYR:HA	1:A:538:VAL:CG2	2.26	0.62
8:P:276:GLU:OE1	8:P:319:PHE:HZ	1.83	0.62
9:a:503:LEU:HD13	9:a:528:ASN:ND2	2.13	0.62
13:s:359:VAL:HG12	13:s:359:VAL:O	2.00	0.62
12:e:41:LEU:N	12:e:41:LEU:HD22	2.14	0.62
15:l:76:ILE:HG23	15:l:92:GLN:HE21	1.65	0.62
1:A:523:ASN:O	1:A:526:THR:HG22	2.00	0.61
1:B:263:LEU:CA	1:B:267:SER:OG	2.48	0.61
3:G:54:LEU:HD22	3:G:118:LEU:HG	1.82	0.61
5:K:152:ILE:N	5:K:153:PRO:CD	2.61	0.61
5:J:164:ASP:O	5:J:165:VAL:C	2.42	0.61
9:a:410:LEU:HB3	9:a:467:CYS:HB2	1.82	0.61
1:B:17:THR:CG2	1:B:18:PHE:CE1	2.81	0.61
7:O:113:ASN:ND2	7:O:113:ASN:H	1.97	0.61
1:A:264:SER:O	1:A:308:ARG:NH2	2.34	0.61
9:a:481:VAL:CB	9:a:510:VAL:HA	2.30	0.61
9:a:486:ASP:O	9:a:489:ASN:O	2.17	0.61
10:b:19:LEU:HD12	19:g:201:POV:H37	1.83	0.61
15:k:45:SER:HB2	15:k:52:ILE:HD11	1.82	0.61
4:H:74:PHE:HZ	11:d:348:ILE:HD12	1.64	0.61
1:C:197:GLU:H	1:C:199:ILE:HG22	1.66	0.61
2:E:380:ASP:HB2	2:E:393:ASN:HB2	1.83	0.61
9:a:526:ALA:CA	12:e:68:LEU:HD23	2.29	0.61
9:a:496:ARG:HH21	12:e:70:ASN:ND2	1.65	0.60
1:C:76:GLY:HA3	7:M:113:ASN:CG	2.25	0.60
2:E:177:ILE:HD11	2:E:392:ILE:HD13	1.82	0.60
8:P:335:ASP:O	8:P:339:SER:N	2.33	0.60
9:a:506:ALA:HB3	9:a:600:ALA:CB	2.31	0.60
15:o:44:MET:HG3	15:o:122:ALA:HB2	1.83	0.60
1:B:459:ARG:NH2	2:D:468:TYR:OH	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:PHE:HE2	1:A:476:ARG:NH2	1.98	0.60
5:J:180:GLY:HA3	5:J:195:THR:HA	1.83	0.60
13:s:281:GLU:CG	13:s:315:PHE:CE1	2.85	0.60
13:s:253:VAL:HG21	13:s:266:LEU:HD12	1.82	0.60
13:s:268:TRP:CZ3	13:s:270:GLN:NE2	2.56	0.60
13:s:364:ILE:HG22	13:s:364:ILE:O	2.01	0.60
8:P:334:PHE:O	8:P:338:SER:N	2.32	0.60
1:A:534:PHE:HE1	1:A:537:THR:HB	1.62	0.60
1:B:260:SER:HB2	1:B:263:LEU:HD21	1.84	0.60
14:r:329:ILE:HG22	14:r:329:ILE:O	2.00	0.60
3:G:27:THR:HG22	3:G:35:SER:HB2	1.84	0.59
2:D:167:GLU:HG3	2:D:168:GLU:HG2	1.82	0.59
2:E:285:LEU:O	2:E:289:CYS:O	2.20	0.59
4:H:71:GLU:OE2	4:H:130:GLN:HG3	2.02	0.59
7:O:88:GLN:HE22	7:O:92:ARG:HH21	1.51	0.59
13:s:347:SER:CB	13:s:391:TRP:CZ2	2.73	0.59
1:A:191:VAL:HG21	1:A:205:MET:HG3	1.84	0.59
9:a:527:THR:HG22	12:e:67:GLN:O	2.02	0.59
11:d:169:SER:O	11:d:172:ASP:OD1	2.19	0.59
2:D:89:VAL:HG23	2:D:89:VAL:O	2.01	0.58
10:b:77:ILE:HG21	15:q:117:GLY:HA2	1.84	0.58
9:a:482:ARG:HB2	9:a:483:PRO:HD3	0.76	0.58
2:F:89:VAL:O	2:F:89:VAL:HG23	2.03	0.58
7:O:113:ASN:H	7:O:113:ASN:HD22	1.50	0.58
1:A:248:ILE:HD11	1:A:347:MET:HE1	1.84	0.58
4:H:106:LEU:HD21	4:H:158:LEU:HD13	1.85	0.58
19:b:305:POV:H11	13:s:418:GLY:HA2	1.84	0.58
13:s:403:PHE:O	20:s:506:NAG:O4	2.20	0.58
1:B:535:TYR:HH	1:B:592:ASP:CG	2.04	0.58
8:P:329:GLN:HA	8:P:332:SER:CB	2.32	0.58
9:a:522:ILE:CG1	12:e:66:PRO:HG3	2.33	0.58
8:P:68:THR:HG22	8:P:68:THR:O	2.04	0.58
1:C:232:ARG:H	1:C:522:GLN:HE22	1.52	0.58
5:K:163:VAL:HG23	5:K:163:VAL:O	1.99	0.58
9:a:484:MET:HE2	9:a:509:GLY:HA3	1.86	0.58
15:o:72:VAL:HG21	15:o:99:VAL:HG11	1.84	0.58
9:a:612:HIS:HD2	9:a:633:GLN:HE22	1.52	0.58
1:A:220:LYS:HA	1:A:392:VAL:HG23	1.84	0.58
1:B:376:ALA:HB1	2:D:309:GLU:HA	1.86	0.58
1:B:17:THR:O	1:B:18:PHE:HD1	1.86	0.57
1:C:383:ALA:HB1	2:E:264:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:226:ASN:O	2:D:291:LYS:HB2	2.03	0.57
7:O:110:VAL:HG12	7:O:111:HIS:N	2.17	0.57
9:a:481:VAL:HG22	9:a:484:MET:HB2	1.84	0.57
1:B:588:ASP:H	1:B:591:LYS:HE3	1.68	0.57
9:a:480:SER:HB3	9:a:522:ILE:CD1	2.21	0.57
2:E:300:MET:HB2	2:E:354:LEU:HB3	1.86	0.57
4:H:40:LEU:HB3	4:H:162:ILE:HD11	1.87	0.57
5:K:137:ARG:NH1	5:K:178:ALA:O	2.37	0.57
10:b:32:GLY:O	19:b:301:POV:H33A	2.04	0.57
15:l:57:ILE:HD12	15:l:132:ILE:HD13	1.86	0.57
9:a:180:ILE:HB	9:a:199:GLN:HE22	1.69	0.57
1:A:472:PHE:HE2	1:A:476:ARG:HH22	1.53	0.57
1:B:260:SER:HB2	1:B:263:LEU:CD2	2.35	0.57
4:H:156:VAL:HG23	6:L:105:ILE:CD1	2.35	0.57
1:A:534:PHE:CD1	1:A:537:THR:HB	2.39	0.57
13:s:354:PHE:CZ	13:s:391:TRP:O	2.55	0.57
1:A:116:ILE:HD11	2:D:287:TYR:CD2	2.40	0.57
4:H:92:VAL:HG22	4:H:113:HIS:HD2	1.68	0.57
11:d:67:VAL:HG21	11:d:334:GLU:HG3	1.86	0.57
15:p:44:MET:HG3	15:p:122:ALA:HB2	1.86	0.57
13:s:274:VAL:HG21	13:s:321:PHE:CE1	2.40	0.57
15:k:72:VAL:HG21	15:k:99:VAL:HG11	1.86	0.57
15:n:124:GLN:NE2	15:o:45:SER:O	2.38	0.57
15:p:72:VAL:HG21	15:p:99:VAL:HG11	1.86	0.57
2:E:445:THR:HG22	2:E:447:ASP:H	1.69	0.56
4:H:85:GLN:HG2	11:d:120:ARG:HH11	1.70	0.56
9:a:527:THR:HG23	12:e:67:GLN:HE21	1.70	0.56
11:d:108:ASN:ND2	11:d:133:GLY:O	2.38	0.56
1:A:523:ASN:HB3	1:A:526:THR:CG2	2.35	0.56
1:B:133:TRP:HB2	1:B:205:MET:HE1	1.86	0.56
1:B:220:LYS:HA	1:B:392:VAL:HG23	1.86	0.56
4:H:69:LEU:HD12	4:H:134:LEU:CD2	2.35	0.56
11:d:224:THR:HG21	11:d:255:LEU:HD22	1.86	0.56
12:e:79:LEU:CD1	16:f:36:HIS:HB2	2.35	0.56
1:B:583:SER:HA	1:B:586:PHE:CE2	2.40	0.56
2:F:82:ARG:HD3	2:F:100:GLU:HB2	1.88	0.56
3:G:241:ALA:HB1	3:G:246:PHE:HB2	1.87	0.56
5:I:180:GLY:HA3	5:I:195:THR:HA	1.87	0.56
9:a:482:ARG:NE	9:a:482:ARG:CA	2.68	0.56
12:e:78:PHE:N	12:e:78:PHE:CD2	2.72	0.56
1:C:138:CYS:C	1:C:140:ASN:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:457:LYS:HB3	2:E:483:LEU:HD22	1.88	0.56
1:B:531:PHE:C	1:B:531:PHE:CD2	2.84	0.56
4:H:71:GLU:OE2	4:H:130:GLN:CG	2.53	0.56
2:E:250:GLU:OE1	5:K:66:GLN:NE2	2.38	0.56
5:J:152:ILE:HG23	5:J:163:VAL:HG21	1.87	0.56
8:P:368:LYS:HB3	8:P:372:LEU:HB2	1.88	0.56
9:a:224:PHE:O	9:a:225:GLN:HG3	2.06	0.56
2:E:229:ILE:HB	2:E:257:VAL:HG22	1.88	0.56
2:F:86:VAL:HG22	2:F:96:VAL:HG12	1.87	0.56
5:J:97:GLU:OE1	7:N:92:ARG:NH2	2.38	0.56
9:a:595:TRP:CZ2	12:e:58:ALA:HB2	2.40	0.56
13:s:325:LEU:HD22	13:s:402:ALA:CB	2.35	0.56
13:s:342:ASN:ND2	13:s:355:ASN:OD1	2.38	0.56
13:s:358:GLN:HB3	13:s:381:LEU:HD22	1.87	0.56
1:A:472:PHE:CE2	1:A:476:ARG:NH2	2.74	0.56
2:F:131:VAL:HG12	2:F:259:LEU:HB3	1.88	0.56
4:H:107:PRO:HD2	4:H:157:THR:HG21	1.88	0.56
6:L:90:GLU:OE1	6:L:101:ALA:CB	2.53	0.56
1:A:430:GLN:HB3	1:A:456:LYS:HB2	1.87	0.56
11:d:299:VAL:HB	11:d:350:ILE:HD13	1.87	0.56
4:H:40:LEU:HD23	4:H:162:ILE:HG13	1.87	0.55
2:D:208:ARG:NH2	2:D:467:PRO:O	2.39	0.55
2:D:492:LEU:HD23	2:D:495:ILE:HD12	1.87	0.55
2:E:123:VAL:HG12	2:E:281:THR:HG22	1.88	0.55
2:F:485:ARG:NH1	2:F:506:ARG:O	2.39	0.55
15:c:44:MET:HE2	15:c:122:ALA:HB2	1.87	0.55
1:A:532:CYS:SG	1:A:536:LYS:CB	2.89	0.55
2:F:300:MET:HB2	2:F:354:LEU:HB3	1.88	0.55
6:L:17:VAL:HG11	6:L:38:VAL:HG22	1.87	0.55
9:a:525:ILE:HG23	12:e:68:LEU:HD21	1.87	0.55
10:b:19:LEU:HD13	10:b:19:LEU:C	2.29	0.55
1:A:138:CYS:HB3	1:A:141:LEU:HB2	1.88	0.55
2:F:233:ALA:HB3	2:F:261:LEU:HA	1.87	0.55
1:B:249:PRO:HB2	1:B:412:PRO:HA	1.89	0.55
13:s:316:GLY:HA3	20:s:504:NAG:H3	1.88	0.55
1:C:258:VAL:HA	1:C:261:GLN:HG2	1.89	0.55
5:I:162:ASP:N	5:I:162:ASP:OD1	2.35	0.55
9:a:525:ILE:HG23	12:e:68:LEU:HD22	1.89	0.55
1:B:17:THR:O	1:B:18:PHE:CD1	2.60	0.55
9:a:71:GLU:HG2	9:a:108:LEU:HD13	1.89	0.55
1:B:66:VAL:HG12	1:B:68:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:m:124:GLN:NE2	15:n:45:SER:O	2.40	0.55
3:G:187:VAL:HG12	3:G:248:VAL:HG22	1.89	0.55
9:a:496:ARG:NE	12:e:70:ASN:HD22	1.84	0.55
4:H:40:LEU:HB3	4:H:162:ILE:HG12	1.89	0.54
11:d:89:ALA:C	11:d:90:TYR:O	2.43	0.54
12:e:75:TYR:C	12:e:75:TYR:CD2	2.84	0.54
13:s:279:HIS:HB2	13:s:315:PHE:HE1	1.72	0.54
1:C:197:GLU:HA	1:C:197:GLU:OE1	2.07	0.54
5:K:180:GLY:HA3	5:K:195:THR:HA	1.89	0.54
9:a:69:GLU:OE2	9:a:73:ARG:NH1	2.40	0.54
13:s:265:ILE:HG13	13:s:265:ILE:O	2.08	0.54
10:b:58:ILE:HG12	15:q:148:VAL:HG11	1.89	0.54
13:s:325:LEU:HD11	13:s:400:ILE:HD11	1.89	0.54
1:A:481:GLU:OE2	1:A:484:GLN:NE2	2.40	0.54
2:E:389:TYR:HB3	2:E:390:PRO:HD2	1.89	0.54
9:a:412:HIS:CE1	9:a:468:PHE:CE2	2.95	0.54
11:d:272:PRO:HA	11:d:275:LYS:HG2	1.89	0.54
1:A:226:PRO:HA	1:A:241:VAL:HA	1.88	0.54
10:b:24:ILE:HG22	19:g:201:POV:H28A	1.90	0.54
10:b:39:TRP:CH2	13:s:420:PHE:O	2.58	0.54
15:l:148:VAL:HG11	15:m:23:MET:HG2	1.89	0.54
1:A:220:LYS:O	2:F:242:ARG:NH2	2.40	0.54
4:H:40:LEU:HD23	4:H:162:ILE:HG12	1.88	0.54
9:a:481:VAL:CG1	9:a:510:VAL:CG2	2.86	0.54
12:e:79:LEU:HD11	16:f:36:HIS:HB2	1.90	0.54
15:k:124:GLN:NE2	15:l:45:SER:O	2.37	0.54
15:n:79:SER:OG	15:n:88:ARG:NH2	2.41	0.54
3:G:4:PHE:HA	3:G:323:PRO:HB3	1.90	0.54
13:s:365:TYR:CD1	13:s:412:TYR:HB3	2.43	0.54
1:B:17:THR:HG22	1:B:17:THR:O	2.07	0.54
4:H:83:VAL:O	4:H:119:TYR:OH	2.25	0.54
9:a:495:LEU:HD22	12:e:74:TRP:HD1	1.71	0.54
2:E:233:ALA:HB3	2:E:261:LEU:HB2	1.90	0.54
2:D:73:HIS:HB2	2:D:113:GLU:HB3	1.90	0.53
3:G:18:THR:HG22	3:G:21:LYS:HG2	1.89	0.53
9:a:481:VAL:HG22	9:a:481:VAL:O	2.08	0.53
10:b:34:ARG:NH2	19:b:304:POV:H14	2.22	0.53
1:A:99:PHE:HB3	1:A:103:GLN:HA	1.90	0.53
1:A:269:SER:O	1:A:308:ARG:NH1	2.41	0.53
1:A:523:ASN:HB3	1:A:526:THR:HG21	1.89	0.53
10:b:47:PHE:O	10:b:51:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:162:ILE:HG22	4:H:162:ILE:O	2.08	0.53
7:M:70:SER:CA	7:M:74:GLU:OE1	2.56	0.53
5:K:32:ALA:HB1	8:P:231:LEU:HD21	1.91	0.53
9:a:482:ARG:CB	9:a:482:ARG:NH1	2.71	0.53
13:s:271:ASN:HB3	13:s:396:ARG:HB2	1.91	0.53
13:s:281:GLU:CG	13:s:315:PHE:CE2	2.84	0.53
14:r:330:TRP:CD1	14:r:330:TRP:C	2.85	0.53
15:q:44:MET:HE2	15:q:122:ALA:HB2	1.91	0.53
9:a:47:PHE:HA	9:a:52:VAL:HG11	1.90	0.53
1:C:105:PRO:HD3	1:C:126:ALA:HA	1.89	0.53
2:E:74:LEU:HD13	2:E:112:CYS:HB3	1.91	0.53
6:L:9:ALA:HB2	6:L:61:ILE:HD12	1.91	0.53
9:a:482:ARG:N	9:a:482:ARG:CD	2.72	0.53
10:b:84:PRO:HG3	15:q:124:GLN:HE22	1.73	0.53
9:a:47:PHE:O	9:a:48:GLN:HG2	2.08	0.53
13:s:335:ARG:HG3	19:g:201:POV:H13B	1.90	0.53
1:A:534:PHE:CD1	1:A:534:PHE:O	2.62	0.53
1:B:68:GLU:OE2	1:B:104:ARG:NH1	2.42	0.53
1:C:372:SER:HB3	1:C:420:PRO:HG3	1.90	0.53
10:b:36:ASP:HB3	10:b:39:TRP:HB3	1.91	0.53
2:F:89:VAL:O	2:F:89:VAL:CG2	2.56	0.53
10:b:122:ASP:OD2	20:s:505:NAG:H81	2.08	0.53
1:A:431:VAL:CG2	1:A:457:TYR:HD2	2.22	0.53
1:C:204:SER:OG	1:C:205:MET:N	2.41	0.53
8:P:284:ARG:HD3	8:P:287:TYR:HE2	1.67	0.53
1:A:465:TYR:O	1:A:470:THR:N	2.38	0.52
1:C:522:GLN:HG3	1:C:529:ASP:HB3	1.91	0.52
3:G:27:THR:O	3:G:30:ASN:ND2	2.42	0.52
10:b:41:LEU:O	10:b:135:TYR:OH	2.26	0.52
9:a:6:ARG:HH22	9:a:558:PHE:HB3	1.74	0.52
15:n:26:SER:OG	15:n:65:ILE:O	2.28	0.52
1:A:266:TYR:OH	1:A:530:ARG:NH1	2.42	0.52
11:d:8:TYR:O	11:d:9:PHE:HB3	2.08	0.52
15:o:79:SER:OG	15:o:88:ARG:NH2	2.42	0.52
1:B:264:SER:O	1:B:308:ARG:NH2	2.43	0.52
5:J:150:LYS:O	5:J:153:PRO:CG	2.58	0.52
9:a:311:ASN:HB2	9:a:320:ILE:H	1.73	0.52
9:a:496:ARG:HH21	12:e:70:ASN:HB3	1.74	0.52
15:m:88:ARG:NH1	15:m:155:LYS:O	2.42	0.52
2:D:197:LEU:HD21	2:D:381:ARG:HG3	1.92	0.52
8:P:66:LEU:N	8:P:66:LEU:CD2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:345:ILE:HG21	13:s:391:TRP:CE3	2.44	0.52
2:D:67:ARG:HB2	2:D:70:GLU:HG3	1.92	0.52
2:D:228:ALA:HA	2:D:256:ASN:HB2	1.92	0.52
2:F:77:PRO:HG3	2:F:106:ASP:HB2	1.90	0.52
9:a:824:LEU:HG	9:a:824:LEU:O	2.09	0.52
3:G:47:THR:HG23	3:G:51:LEU:HB2	1.91	0.52
9:a:406:MET:HA	9:a:746:SER:HB2	1.92	0.52
1:B:248:ILE:HG22	1:B:433:TRP:HB2	1.90	0.52
2:E:318:PRO:HG2	4:H:201:ARG:HD2	1.91	0.52
2:E:390:PRO:O	2:E:391:PRO:C	2.49	0.52
5:J:137:ARG:NH1	5:J:178:ALA:O	2.43	0.52
8:P:260:LYS:HG3	8:P:262:LYS:HG2	1.91	0.52
8:P:131:ASN:HA	8:P:138:VAL:HG12	1.91	0.52
8:P:218:GLY:O	8:P:222:GLN:NE2	2.43	0.52
10:b:56:LEU:HD21	13:s:433:PHE:HZ	1.74	0.52
1:A:21:VAL:HG12	1:A:23:GLY:H	1.75	0.51
1:C:69:GLU:HG2	1:C:319:PRO:HG3	1.91	0.51
1:C:511:VAL:HG11	1:C:548:TYR:HB2	1.92	0.51
3:G:56:ASP:OD2	9:a:232:ARG:NH2	2.43	0.51
6:L:91:ILE:O	6:L:91:ILE:HG13	2.09	0.51
9:a:200:ALA:HB3	9:a:219:VAL:HB	1.91	0.51
9:a:520:ASP:N	9:a:520:ASP:OD1	2.41	0.51
2:D:249:GLU:N	2:D:254:MET:HE2	2.25	0.51
5:J:182:GLU:HG2	5:J:193:SER:HA	1.92	0.51
6:L:70:ILE:HA	6:L:73:MET:HE3	1.90	0.51
15:m:44:MET:HG3	15:m:122:ALA:HB2	1.93	0.51
1:A:277:CYS:HG	1:A:326:SER:HG	1.57	0.51
1:B:416:ASP:OD1	1:B:416:ASP:N	2.43	0.51
4:H:70:ALA:HB1	11:d:334:GLU:OE1	2.11	0.51
8:P:243:ARG:NH1	8:P:285:GLN:OE1	2.43	0.51
9:a:71:GLU:OE2	9:a:112:ASN:ND2	2.44	0.51
11:d:137:GLN:C	11:d:138:MET:HG2	2.35	0.51
2:F:164:ILE:HG23	2:F:340:ARG:HG3	1.93	0.51
5:J:152:ILE:O	5:J:152:ILE:HG22	2.09	0.51
9:a:482:ARG:HB3	12:e:77:ARG:HG2	1.91	0.51
9:a:776:LEU:HA	9:a:779:ILE:HB	1.91	0.51
13:s:338:PHE:HZ	13:s:367:PHE:HB2	1.75	0.51
15:c:115:ASP:OD1	15:c:119:ARG:NH1	2.44	0.51
2:E:128:LEU:HD23	2:E:258:CYS:HB2	1.93	0.51
1:A:204:SER:OG	1:A:205:MET:N	2.39	0.51
2:E:171:GLN:HB3	2:E:211:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:NZ	1:A:584:MET:O	2.42	0.51
1:B:383:ALA:HB1	2:D:264:ALA:HB1	1.92	0.51
1:B:482:ILE:HG22	1:B:512:ALA:HB2	1.92	0.51
3:G:218:GLU:HA	3:G:223:TYR:HA	1.93	0.51
5:J:128:LEU:HD22	5:J:161:ARG:NH2	2.25	0.51
9:a:36:GLN:HB3	9:a:324:TRP:HB2	1.93	0.51
1:A:30:THR:HA	1:A:63:THR:HA	1.93	0.51
2:E:124:SER:H	2:E:127:MET:HE2	1.74	0.51
9:a:752:LEU:HD22	9:a:791:LEU:HD13	1.93	0.51
15:k:41:ILE:HD13	15:k:118:VAL:HG11	1.92	0.51
1:A:531:PHE:CD1	1:A:531:PHE:C	2.84	0.51
7:O:113:ASN:ND2	7:O:113:ASN:N	2.59	0.51
12:e:41:LEU:N	12:e:41:LEU:CD2	2.73	0.51
15:k:51:MET:HG3	15:k:54:LYS:HD3	1.92	0.51
9:a:114:ASN:O	9:a:118:LEU:HB2	2.11	0.51
11:d:272:PRO:HG3	15:g:123:GLN:HA	1.92	0.51
3:G:222:SER:OG	3:G:223:TYR:N	2.45	0.50
4:H:74:PHE:HZ	11:d:348:ILE:CD1	2.24	0.50
2:D:124:SER:H	2:D:127:MET:HE2	1.76	0.50
13:s:345:ILE:CD1	13:s:393:MET:CE	2.85	0.50
15:q:82:ASP:N	15:q:82:ASP:OD1	2.42	0.50
2:D:168:GLU:OE2	2:D:215:LYS:NZ	2.45	0.50
6:L:44:THR:HG23	6:L:47:GLU:H	1.76	0.50
8:P:69:GLU:O	8:P:70:GLY:C	2.53	0.50
4:H:69:LEU:CD1	4:H:134:LEU:CD2	2.83	0.50
4:H:87:VAL:HG11	6:L:21:LEU:HD22	1.93	0.50
7:M:110:VAL:C	7:M:111:HIS:O	2.41	0.50
11:d:83:ARG:NH2	11:d:131:PRO:O	2.44	0.50
1:A:46:GLY:HA2	1:A:77:ASP:HB3	1.92	0.50
2:E:443:ALA:HB1	2:E:444:LEU:HD23	1.94	0.50
4:H:40:LEU:HD21	4:H:104:VAL:HG21	1.94	0.50
5:I:202:LEU:O	5:I:206:GLN:NE2	2.44	0.50
2:D:271:ARG:HD2	2:D:306:ALA:HB2	1.94	0.50
2:E:193:SER:OG	2:E:194:ALA:N	2.43	0.50
5:I:55:GLU:HA	5:I:58:GLU:HB2	1.93	0.50
7:M:110:VAL:HG23	7:M:111:HIS:O	2.12	0.50
9:a:89:PRO:HG2	9:a:300:MET:HE3	1.94	0.50
1:C:598:LYS:HA	1:C:601:TYR:HB3	1.94	0.50
2:D:288:GLN:O	5:J:222:ARG:HA	2.12	0.50
10:b:16:TRP:O	10:b:19:LEU:N	2.43	0.50
12:e:37:ILE:O	12:e:41:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:TYR:CZ	1:B:586:PHE:HD1	2.30	0.50
6:L:32:ARG:O	6:L:33:HIS:ND1	2.44	0.50
2:D:187:GLN:HG3	2:D:401:LEU:HD12	1.94	0.49
3:G:263:GLU:O	3:G:267:ARG:N	2.45	0.49
11:d:121:SER:CB	11:d:145:GLN:HG2	2.42	0.49
6:L:75:ARG:HE	6:L:78:LEU:HD11	1.77	0.49
8:P:279:VAL:C	8:P:280:GLU:HG3	2.36	0.49
2:E:233:ALA:O	2:E:262:ASN:N	2.43	0.49
2:F:82:ARG:NH1	2:F:101:GLY:O	2.45	0.49
9:a:453:MET:HE1	9:a:800:PHE:HD1	1.76	0.49
9:a:527:THR:CG2	12:e:67:GLN:HG2	2.43	0.49
12:e:78:PHE:N	12:e:78:PHE:HD2	2.10	0.49
1:A:43:VAL:HG21	1:A:64:ILE:HD13	1.93	0.49
2:D:395:LEU:HA	2:D:423:TYR:HE1	1.77	0.49
10:b:23:GLY:HA2	19:g:201:POV:H34	1.94	0.49
10:b:40:PHE:CD1	13:s:425:TRP:NE1	2.80	0.49
2:F:436:LYS:HB3	2:F:444:LEU:HD21	1.94	0.49
9:a:28:GLU:OE2	9:a:339:ARG:NH1	2.45	0.49
10:b:20:LEU:HD12	19:g:201:POV:H311	1.94	0.49
11:d:110:ILE:HD12	11:d:181:ILE:HG23	1.95	0.49
1:B:430:GLN:NE2	2:D:237:ASN:OD1	2.46	0.49
9:a:444:PHE:O	9:a:447:ARG:NH1	2.44	0.49
9:a:652:LEU:HA	9:a:655:LYS:HE2	1.94	0.49
11:d:113:ILE:HG22	11:d:151:TYR:HE2	1.76	0.49
1:A:266:TYR:OH	1:A:530:ARG:CZ	2.61	0.49
1:C:226:PRO:HA	1:C:241:VAL:HA	1.95	0.49
9:a:503:LEU:HD11	9:a:528:ASN:HD21	1.72	0.49
10:b:19:LEU:C	10:b:19:LEU:CD1	2.85	0.49
11:d:15:TYR:OH	15:q:123:GLN:NE2	2.44	0.49
2:D:192:PHE:HB3	2:D:356:MET:HE3	1.95	0.48
8:P:294:CYS:SG	8:P:295:LYS:N	2.86	0.48
1:B:226:PRO:HA	1:B:241:VAL:HA	1.95	0.48
2:D:247:ASP:OD1	2:D:247:ASP:C	2.46	0.48
4:H:40:LEU:HB3	4:H:162:ILE:CG1	2.43	0.48
5:J:150:LYS:O	5:J:153:PRO:HD2	2.12	0.48
1:A:23:GLY:HA2	2:D:89:VAL:O	2.12	0.48
1:B:492:ILE:HG23	2:D:438:VAL:HG12	1.96	0.48
1:C:76:GLY:HA3	7:M:113:ASN:OD1	2.13	0.48
4:H:123:GLY:O	4:H:124:LEU:HB3	2.13	0.48
9:a:498:ASN:CB	9:a:499:PRO:HD3	2.36	0.48
1:A:266:TYR:OH	1:A:530:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:TYR:HB2	1:B:588:ASP:OD1	2.08	0.48
9:a:176:ASN:HA	9:a:217:LYS:HA	1.94	0.48
9:a:526:ALA:HB2	12:e:66:PRO:HB2	1.95	0.48
13:s:325:LEU:HD22	13:s:402:ALA:HB2	1.96	0.48
2:F:183:ILE:HG22	2:F:189:ILE:HD13	1.95	0.48
11:d:83:ARG:O	11:d:87:ASN:ND2	2.46	0.48
15:m:148:VAL:HG11	15:n:23:MET:HG2	1.95	0.48
5:J:199:ARG:HH21	7:N:103:VAL:HA	1.79	0.48
9:a:484:MET:CE	9:a:509:GLY:HA3	2.43	0.48
15:n:148:VAL:HG11	15:o:23:MET:HG2	1.95	0.48
2:E:87:LEU:HD13	2:E:314:ARG:HD2	1.95	0.48
9:a:501:LEU:HD13	9:a:527:THR:HG21	1.95	0.48
1:B:90:LEU:HB2	1:B:207:GLN:HG3	1.96	0.48
18:C:702:ADP:O2B	2:F:400:ARG:NH1	2.46	0.48
2:D:124:SER:OG	2:D:125:GLU:N	2.47	0.48
5:K:154:VAL:O	5:K:157:VAL:HG22	2.13	0.48
9:a:495:LEU:HD12	9:a:495:LEU:HA	1.47	0.48
12:e:74:TRP:HA	12:e:77:ARG:HG3	1.95	0.48
14:r:338:SER:HA	15:n:123:GLN:HE22	1.77	0.48
15:l:82:ASP:N	15:l:82:ASP:OD1	2.45	0.48
15:q:88:ARG:NH2	15:q:155:LYS:OXT	2.47	0.48
1:A:431:VAL:CG2	1:A:457:TYR:CD2	2.97	0.48
1:B:574:MET:HE1	1:B:609:GLN:HB3	1.96	0.48
2:F:133:ASN:HB3	2:F:139:ILE:HD11	1.94	0.48
9:a:36:GLN:O	9:a:323:VAL:HA	2.14	0.48
9:a:482:ARG:HA	9:a:482:ARG:CZ	2.43	0.48
11:d:110:ILE:HG13	11:d:182:ARG:HG2	1.95	0.48
13:s:347:SER:OG	13:s:350:SER:OG	2.32	0.48
1:B:295:THR:HA	1:B:304:SER:HA	1.95	0.48
4:H:13:ARG:HD2	4:H:191:LEU:HD13	1.94	0.48
8:P:287:TYR:O	8:P:291:MET:N	2.46	0.48
9:a:79:ILE:HG21	9:a:290:ILE:HD11	1.96	0.48
9:a:482:ARG:NH1	9:a:482:ARG:CG	2.72	0.48
9:a:805:ARG:HH21	15:n:136:ILE:HD12	1.79	0.48
19:r:401:POV:H3	15:o:10:TYR:HB3	1.96	0.48
1:B:105:PRO:HD3	1:B:126:ALA:HA	1.95	0.47
1:C:231:GLN:HB2	1:C:234:LEU:HB2	1.96	0.47
1:C:369:PRO:O	4:H:201:ARG:NH1	2.47	0.47
2:E:188:LYS:NZ	2:E:374:GLU:OE2	2.43	0.47
4:H:89:LYS:HA	6:L:27:GLU:HG2	1.96	0.47
9:a:527:THR:HG22	12:e:67:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:336:GLU:O	8:P:340:GLU:N	2.42	0.47
8:P:427:ASP:HB3	8:P:430:VAL:HG22	1.95	0.47
13:s:296:THR:OG1	13:s:297:GLY:N	2.47	0.47
1:B:587:LYS:HA	1:B:591:LYS:HE3	1.96	0.47
2:D:129:GLY:HA2	2:D:254:MET:HG3	1.95	0.47
4:H:111:HIS:HB3	4:H:146:VAL:HG11	1.97	0.47
13:s:404:ASN:HD22	20:s:506:NAG:C4	2.18	0.47
4:H:43:ARG:HH11	4:H:101:VAL:HB	1.79	0.47
9:a:482:ARG:NH2	12:e:73:ILE:HB	2.30	0.47
10:b:200:ARG:NH2	15:c:77:ALA:O	2.44	0.47
11:d:262:GLU:O	11:d:266:ASN:ND2	2.48	0.47
2:D:191:ILE:HB	2:D:353:ILE:HG12	1.95	0.47
3:G:179:SER:O	3:G:180:GLU:C	2.58	0.47
5:K:152:ILE:O	5:K:152:ILE:CG2	2.60	0.47
8:P:305:GLN:HB3	9:a:53:ASN:HD21	1.80	0.47
9:a:522:ILE:HD11	12:e:68:LEU:HD11	1.96	0.47
9:a:769:SER:OG	9:a:770:LEU:N	2.47	0.47
15:o:72:VAL:HA	15:o:75:LEU:HB2	1.96	0.47
1:A:277:CYS:SG	1:A:326:SER:OG	2.68	0.47
4:H:121:LEU:HB3	4:H:124:LEU:HD22	1.95	0.47
13:s:420:PHE:HB3	13:s:425:TRP:HB2	1.95	0.47
15:q:77:ALA:HA	15:q:80:LEU:HD12	1.96	0.47
1:B:139:LYS:O	1:B:139:LYS:HG2	2.15	0.47
1:C:156:VAL:O	1:C:164:HIS:N	2.46	0.47
2:E:288:GLN:O	5:K:223:LYS:N	2.42	0.47
2:F:488:PRO:HD2	2:F:491:MET:HE2	1.97	0.47
3:G:32:LEU:HD11	3:G:330:LYS:HG3	1.97	0.47
4:H:91:GLN:HG2	4:H:115:GLY:HA2	1.96	0.47
4:H:145:LEU:HD12	6:L:89:LEU:HD22	1.97	0.47
5:J:153:PRO:O	5:J:157:VAL:CG2	2.58	0.47
8:P:279:VAL:O	8:P:280:GLU:CG	2.58	0.47
9:a:481:VAL:HG13	9:a:510:VAL:CG2	2.45	0.47
9:a:652:LEU:HD21	9:a:722:ALA:HA	1.96	0.47
12:e:79:LEU:CD1	16:f:36:HIS:CB	2.92	0.47
13:s:355:ASN:O	13:s:382:LEU:HA	2.15	0.47
2:E:388:ILE:HG23	2:E:464:ALA:HB2	1.97	0.47
9:a:459:TYR:OH	12:e:48:CYS:O	2.26	0.47
11:d:107:ASP:OD1	11:d:182:ARG:NH2	2.46	0.47
13:s:322:LYS:HB2	13:s:344:GLU:HB2	1.95	0.47
2:D:210:ALA:HB3	2:D:229:ILE:HD11	1.97	0.47
2:F:395:LEU:O	2:F:423:TYR:OH	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:8:ILE:HG23	6:L:63:ILE:HB	1.96	0.47
9:a:15:LEU:HB2	9:a:321:ALA:HB3	1.97	0.47
10:b:34:ARG:HH21	19:b:304:POV:C14	2.27	0.47
10:b:54:ILE:HG12	10:b:111:ILE:HG23	1.97	0.47
15:l:23:MET:HE3	15:l:27:ALA:HB2	1.96	0.47
1:A:531:PHE:CG	1:A:531:PHE:O	2.66	0.47
1:B:134:ASP:OD1	1:B:134:ASP:N	2.38	0.47
2:E:133:ASN:HB3	2:E:139:ILE:HD11	1.97	0.47
3:G:23:HIS:O	3:G:26:THR:OG1	2.29	0.47
8:P:345:ARG:O	8:P:388:VAL:HG11	2.15	0.46
13:s:306:ARG:HG2	13:s:324:ILE:HD13	1.96	0.46
15:q:33:GLY:O	15:q:37:SER:OG	2.27	0.46
1:C:17:THR:HB	1:C:18:PHE:CD2	2.51	0.46
2:F:438:VAL:HG13	2:F:439:VAL:HG23	1.97	0.46
3:G:68:VAL:HA	3:G:71:LYS:HE2	1.97	0.46
5:J:208:MET:HA	5:J:211:VAL:HG22	1.96	0.46
6:L:40:GLU:O	6:L:43:THR:HG22	2.15	0.46
9:a:131:ILE:HG22	9:a:219:VAL:HG22	1.96	0.46
1:A:508:THR:HG22	1:A:548:TYR:HE1	1.80	0.46
1:C:349:ASP:HA	1:C:350:SER:HA	1.65	0.46
2:E:188:LYS:HE2	2:E:336:GLU:HA	1.97	0.46
3:G:264:GLU:HG2	3:G:268:LEU:HG	1.96	0.46
9:a:357:THR:OG1	9:a:358:ASN:N	2.47	0.46
9:a:482:ARG:CB	9:a:483:PRO:CD	2.41	0.46
12:e:24:GLY:C	12:e:26:TRP:N	2.70	0.46
15:g:14:PHE:HB3	15:g:93:LEU:HD22	1.97	0.46
1:B:263:LEU:C	1:B:263:LEU:HD12	2.41	0.46
2:D:186:GLY:H	2:D:349:THR:HB	1.80	0.46
7:M:82:GLN:HA	7:M:85:GLN:HB2	1.97	0.46
9:a:127:GLU:OE2	9:a:245:TYR:OH	2.34	0.46
11:d:90:TYR:O	11:d:94:ALA:HB2	2.15	0.46
13:s:270:GLN:HE21	13:s:270:GLN:N	2.13	0.46
1:A:241:VAL:HG12	1:A:461:LEU:HD21	1.98	0.46
1:C:34:MET:HG3	1:C:81:ARG:HD3	1.97	0.46
1:C:134:ASP:OD1	1:C:134:ASP:N	2.47	0.46
3:G:137:LYS:HD3	3:G:137:LYS:HA	1.76	0.46
9:a:57:ARG:NH2	9:a:94:MET:SD	2.88	0.46
10:b:169:ASN:HB3	10:b:172:LEU:HG	1.98	0.46
13:s:359:VAL:HA	13:s:367:PHE:CZ	2.51	0.46
15:o:106:ALA:HB2	15:o:141:LEU:HB2	1.98	0.46
19:b:303:POV:H29	19:r:402:POV:H35	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:356:ALA:HB2	13:s:382:LEU:CD2	2.45	0.46
15:n:44:MET:HG2	15:n:122:ALA:HB2	1.97	0.46
2:F:130:ARG:NH2	2:F:143:PRO:O	2.42	0.46
7:N:82:GLN:HA	7:N:85:GLN:HG2	1.97	0.46
9:a:65:LEU:HB3	9:a:294:PHE:HE1	1.80	0.46
9:a:507:VAL:HG13	9:a:600:ALA:HB3	1.96	0.46
10:b:59:SER:HB2	15:q:101:LEU:HB3	1.98	0.46
14:r:330:TRP:CD1	14:r:330:TRP:O	2.69	0.46
1:A:471:GLU:O	1:A:471:GLU:HG2	2.16	0.46
5:J:93:ASP:HA	5:J:96:ASN:HB2	1.97	0.46
5:J:174:PRO:HD2	5:J:177:ILE:HD12	1.98	0.46
10:b:91:LEU:HD23	10:b:94:ILE:HG13	1.97	0.46
11:d:17:GLU:OE2	11:d:309:GLN:NE2	2.48	0.46
15:c:64:ILE:HA	15:c:67:ILE:HG12	1.98	0.46
15:k:134:ILE:HG23	15:l:59:VAL:HG11	1.97	0.46
1:A:280:ARG:HB2	1:A:283:GLU:HB2	1.98	0.46
1:A:459:ARG:N	1:A:459:ARG:CD	2.72	0.46
1:B:165:LYS:HD3	1:B:340:MET:HB3	1.98	0.46
1:C:587:LYS:HE3	1:C:591:LYS:HD2	1.98	0.46
2:D:45:LEU:HD11	5:J:126:GLN:HG2	1.97	0.46
4:H:40:LEU:CD2	4:H:162:ILE:HG12	2.46	0.46
5:K:152:ILE:HG23	5:K:163:VAL:HG21	1.97	0.46
9:a:133:ARG:O	9:a:133:ARG:NH1	2.47	0.46
9:a:819:THR:OG1	9:a:820:GLY:N	2.47	0.46
9:a:468:PHE:CE1	16:f:25:MET:HE2	2.51	0.46
2:D:250:GLU:HG3	5:J:70:ILE:HG12	1.98	0.45
9:a:789:ALA:HA	9:a:793:ILE:HD12	1.97	0.45
11:d:230:THR:O	11:d:230:THR:HG23	2.16	0.45
15:g:124:GLN:HE22	15:k:49:PRO:HB3	1.81	0.45
2:D:228:ALA:HB3	2:D:293:VAL:HG22	1.97	0.45
3:G:261:ASP:O	3:G:265:MET:N	2.47	0.45
5:I:122:GLN:HA	7:M:108:PRO:HB3	1.98	0.45
9:a:465:ASN:HB3	9:a:466:ASP:H	1.50	0.45
12:e:10:VAL:HA	12:e:52:TRP:HH2	1.80	0.45
15:m:44:MET:HE2	15:m:44:MET:HB3	1.86	0.45
15:n:44:MET:HE3	15:n:44:MET:HB3	1.90	0.45
1:B:583:SER:HA	1:B:586:PHE:HE2	1.81	0.45
11:d:110:ILE:HD11	11:d:185:LEU:HD12	1.98	0.45
15:g:44:MET:HB2	15:g:122:ALA:HB2	1.98	0.45
1:A:372:SER:HB2	1:A:420:PRO:HG3	1.98	0.45
1:B:74:SER:HB3	2:E:67:ARG:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:VAL:HG22	2:D:96:VAL:HG12	1.97	0.45
2:E:119:LEU:HD23	2:E:153:ILE:HD13	1.99	0.45
2:E:298:THR:HB	2:E:353:ILE:HD12	1.99	0.45
9:a:41:ASN:OD1	9:a:41:ASN:N	2.49	0.45
14:r:304:TYR:OH	19:r:402:POV:O13	2.32	0.45
2:E:71:ILE:HD12	2:E:119:LEU:HD13	1.97	0.45
5:I:81:LEU:HB3	5:I:85:ARG:HH21	1.81	0.45
5:I:93:ASP:HA	5:I:96:ASN:HB2	1.98	0.45
8:P:357:PHE:O	8:P:361:ASN:ND2	2.50	0.45
9:a:479:TRP:CB	9:a:522:ILE:HG21	2.44	0.45
10:b:2:THR:HB	10:b:5:VAL:HB	1.98	0.45
2:F:186:GLY:H	2:F:349:THR:HB	1.82	0.45
3:G:49:ASP:OD1	3:G:49:ASP:N	2.42	0.45
9:a:89:PRO:HD3	9:a:296:LYS:HD2	1.99	0.45
9:a:479:TRP:HE3	9:a:520:ASP:OD2	2.00	0.45
14:r:321:THR:HG23	21:r:403:OLA:H82	1.98	0.45
15:m:118:VAL:HA	15:m:121:THR:HG22	1.97	0.45
2:D:266:ASP:OD1	2:D:266:ASP:N	2.49	0.45
2:E:465:GLN:NE2	2:E:469:GLU:O	2.50	0.45
2:F:388:ILE:HG23	2:F:464:ALA:HB2	1.98	0.45
3:G:270:THR:O	3:G:274:LYS:N	2.47	0.45
9:a:135:THR:HA	9:a:138:PHE:HB3	1.99	0.45
10:b:28:ILE:HD11	15:l:13:PHE:CG	2.51	0.45
11:d:180:ILE:HG23	11:d:240:LEU:HD11	1.99	0.45
11:d:289:THR:OG1	11:d:290:LEU:N	2.49	0.45
1:A:430:GLN:HB2	1:A:457:TYR:CE2	2.52	0.45
1:B:229:THR:OG1	1:B:235:ASP:OD1	2.35	0.45
1:B:511:VAL:HG11	1:B:548:TYR:HB2	1.98	0.45
2:D:445:THR:OG1	2:D:446:SER:N	2.50	0.45
7:M:16:LYS:HA	7:M:19:ALA:HB3	1.99	0.45
8:P:294:CYS:O	8:P:298:LYS:NZ	2.46	0.45
3:G:10:PRO:HB3	3:G:317:GLN:H	1.81	0.45
3:G:153:LEU:HD11	3:G:265:MET:HA	1.99	0.45
4:H:90:ALA:HB2	6:L:27:GLU:HB2	1.99	0.45
5:J:150:LYS:O	5:J:153:PRO:CD	2.65	0.45
15:k:44:MET:HE2	15:k:44:MET:HB3	1.88	0.45
1:A:223:ALA:O	1:A:460:ALA:HB1	2.17	0.45
2:D:127:MET:HE3	2:D:127:MET:HB2	1.75	0.45
2:F:249:GLU:HG2	2:F:254:MET:HG3	1.98	0.45
6:L:90:GLU:CD	6:L:101:ALA:HB3	2.41	0.45
10:b:95:ILE:HA	10:b:98:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:105:MET:HB3	11:d:160:LEU:HD11	1.99	0.45
11:d:213:GLU:HG2	11:d:245:GLY:HA2	1.99	0.45
15:g:77:ALA:HA	15:g:80:LEU:HD12	1.99	0.45
15:p:106:ALA:HB2	15:p:141:LEU:HB2	1.99	0.45
1:C:98:ILE:HG12	1:C:106:LEU:HD12	1.99	0.44
2:D:291:LYS:HE2	2:D:291:LYS:HB3	1.83	0.44
7:N:113:ASN:ND2	7:N:113:ASN:N	2.59	0.44
9:a:178:GLU:O	9:a:179:ARG:NH1	2.50	0.44
9:a:515:TYR:HB2	9:a:520:ASP:HB3	1.99	0.44
2:F:193:SER:O	2:F:355:THR:HA	2.17	0.44
2:F:234:MET:N	2:F:298:THR:O	2.48	0.44
2:F:262:ASN:HD21	2:F:271:ARG:HG2	1.82	0.44
4:H:164:ILE:HG22	4:H:167:ARG:HH21	1.82	0.44
19:b:301:POV:H36A	19:g:201:POV:H3A	1.99	0.44
5:K:90:LEU:HD23	7:O:88:GLN:HG3	1.99	0.44
9:a:131:ILE:HG21	9:a:174:VAL:HG22	1.98	0.44
19:b:301:POV:H27	19:b:301:POV:H39A	1.99	0.44
13:s:364:ILE:HG12	20:s:506:NAG:H83	1.99	0.44
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.46	0.44
1:B:271:VAL:HG23	1:B:344:VAL:HG13	2.00	0.44
2:D:119:LEU:HD23	2:D:153:ILE:HD13	2.00	0.44
13:s:327:ASN:HB2	13:s:403:PHE:CD2	2.53	0.44
1:B:17:THR:C	1:B:18:PHE:CD1	2.96	0.44
1:C:88:VAL:HG11	1:C:329:THR:HG23	1.98	0.44
1:C:352:SER:HB2	1:C:411:SER:H	1.81	0.44
8:P:240:GLU:OE2	8:P:280:GLU:CD	2.60	0.44
8:P:286:GLU:C	8:P:290:ALA:HB3	2.42	0.44
13:s:272:PHE:HD2	13:s:283:LEU:HB2	1.83	0.44
15:o:124:GLN:HE21	15:o:126:ARG:HG3	1.83	0.44
1:C:553:ARG:O	1:C:557:THR:OG1	2.27	0.44
2:E:169:MET:HB2	2:E:405:ALA:HB1	1.99	0.44
2:E:183:ILE:HG12	2:E:189:ILE:HD13	1.99	0.44
7:M:70:SER:HA	7:M:74:GLU:OE1	2.16	0.44
1:A:349:ASP:HA	1:A:350:SER:HA	1.66	0.44
1:A:467:LYS:HE3	1:A:467:LYS:HB3	1.55	0.44
1:C:71:SER:HB3	1:C:120:ARG:HH22	1.83	0.44
2:D:300:MET:HB2	2:D:354:LEU:HB3	2.00	0.44
2:E:205:GLN:HA	2:E:208:ARG:HE	1.81	0.44
4:H:162:ILE:O	4:H:162:ILE:CG2	2.65	0.44
9:a:482:ARG:HH11	9:a:482:ARG:HB3	1.82	0.44
2:D:54:ASN:N	2:D:54:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:200:ARG:NH2	15:c:80:LEU:O	2.50	0.44
11:d:73:ARG:HD2	11:d:73:ARG:HA	1.74	0.44
15:l:44:MET:HG2	15:l:122:ALA:HB2	2.00	0.44
15:n:106:ALA:HB2	15:n:141:LEU:HB2	2.00	0.44
15:o:124:GLN:HG2	15:o:126:ARG:H	1.83	0.44
1:A:298:VAL:HG23	1:A:300:GLY:H	1.83	0.44
1:B:233:VAL:HG23	1:B:237:LEU:HD12	1.99	0.44
1:C:494:GLN:HA	2:F:435:MET:HE1	1.99	0.44
2:D:248:PHE:HE2	2:D:259:LEU:HD13	1.83	0.44
2:D:354:LEU:HD21	2:D:369:THR:HG21	2.00	0.44
2:E:444:LEU:O	2:E:445:THR:OG1	2.32	0.44
8:P:371:GLU:O	8:P:375:ILE:N	2.37	0.44
9:a:481:VAL:HG21	9:a:509:GLY:O	2.18	0.44
9:a:530:LEU:HD21	9:a:751:GLN:HE21	1.82	0.44
13:s:356:ALA:HB2	13:s:382:LEU:HD22	1.99	0.44
15:l:77:ALA:HA	15:l:80:LEU:HD12	2.00	0.44
1:C:565:ILE:HG12	1:C:569:ILE:HD11	2.00	0.43
2:E:413:LYS:HE3	2:E:413:LYS:HB3	1.80	0.43
5:I:155:TYR:CD1	5:I:163:VAL:HG11	2.49	0.43
5:I:215:LEU:HD21	7:M:88:GLN:HG2	2.00	0.43
9:a:537:LYS:HB3	9:a:743:TRP:CD1	2.53	0.43
12:e:56:ILE:O	12:e:59:GLN:N	2.50	0.43
13:s:270:GLN:NE2	13:s:270:GLN:CA	2.71	0.43
13:s:366:SER:O	13:s:414:SER:N	2.34	0.43
1:A:116:ILE:CD1	2:D:287:TYR:CD2	3.01	0.43
2:F:137:LYS:HA	2:F:137:LYS:HD3	1.90	0.43
5:I:208:MET:HA	5:I:211:VAL:HG22	1.99	0.43
9:a:412:HIS:CE1	9:a:468:PHE:CD2	3.06	0.43
9:a:503:LEU:HD11	9:a:528:ASN:ND2	2.31	0.43
15:c:98:SER:O	15:c:102:SER:OG	2.33	0.43
15:k:148:VAL:HA	15:k:151:ILE:HG12	2.00	0.43
1:A:96:GLY:HA2	1:A:306:MET:HG3	2.00	0.43
1:A:535:TYR:O	1:A:536:LYS:C	2.54	0.43
9:a:14:GLN:N	9:a:353:ASN:O	2.48	0.43
1:B:588:ASP:CB	1:B:589:PRO:HD3	2.28	0.43
2:E:321:ARG:HH22	4:H:10:PHE:HE2	1.67	0.43
9:a:122:PHE:HE1	9:a:265:ILE:HG23	1.83	0.43
9:a:134:LYS:O	9:a:138:PHE:N	2.46	0.43
13:s:270:GLN:NE2	13:s:270:GLN:HA	2.33	0.43
15:n:140:VAL:HA	15:n:143:LEU:HB3	1.99	0.43
2:D:374:GLU:O	2:D:400:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:177:ILE:CD1	2:E:392:ILE:HD13	2.48	0.43
3:G:42:ASP:OD1	3:G:42:ASP:N	2.51	0.43
9:a:372:TYR:O	9:a:376:ASN:ND2	2.49	0.43
11:d:93:LEU:HD23	11:d:97:LEU:HG	2.00	0.43
15:m:48:ARG:NH1	15:m:50:GLU:OE2	2.51	0.43
15:q:49:PRO:HA	15:q:52:ILE:HD11	2.00	0.43
5:J:53:ILE:O	5:J:57:TYR:N	2.51	0.43
9:a:112:ASN:OD1	9:a:279:ARG:NH1	2.51	0.43
11:d:9:PHE:O	11:d:9:PHE:CG	2.71	0.43
13:s:358:GLN:NE2	13:s:381:LEU:CD2	2.81	0.43
2:D:421:GLN:NE2	2:D:425:CYS:SG	2.82	0.43
13:s:354:PHE:HE2	13:s:393:MET:HG2	1.84	0.43
1:B:153:TYR:CZ	1:B:192:LEU:HB2	2.53	0.43
1:C:195:GLU:HA	1:C:199:ILE:O	2.18	0.43
1:A:134:ASP:OD1	1:A:134:ASP:N	2.43	0.43
2:F:126:ASP:OD1	5:I:212:ARG:NH2	2.44	0.43
5:J:152:ILE:HG22	5:J:156:LYS:HE3	2.01	0.43
9:a:463:ILE:HG13	12:e:51:PHE:HD2	1.84	0.43
15:p:94:GLY:HA3	15:q:16:VAL:HG22	2.01	0.43
1:B:249:PRO:HG2	1:B:435:LEU:HB2	2.00	0.43
1:B:587:LYS:N	1:B:587:LYS:CD	2.79	0.43
1:B:587:LYS:NZ	1:B:598:LYS:HG2	2.34	0.43
2:D:379:VAL:HG13	2:D:391:PRO:HG2	2.00	0.43
2:E:71:ILE:HG23	2:E:115:THR:HB	2.01	0.43
4:H:70:ALA:CB	11:d:334:GLU:OE1	2.67	0.43
4:H:132:ALA:H	4:H:135:LYS:HG3	1.83	0.43
9:a:7:SER:HB2	9:a:387:ARG:HA	1.99	0.43
9:a:528:ASN:H	12:e:67:GLN:HB3	1.84	0.43
9:a:751:GLN:HB3	15:m:147:ILE:HD12	2.01	0.43
11:d:208:MET:HE1	11:d:316:TYR:HB3	2.01	0.43
15:c:124:GLN:NE2	15:g:45:SER:O	2.51	0.43
15:n:110:ILE:HG23	15:n:135:LEU:HD22	2.01	0.43
15:p:8:PRO:HG2	15:p:11:ALA:HB2	2.01	0.43
2:D:125:GLU:OE2	2:D:291:LYS:NZ	2.51	0.42
7:M:70:SER:HA	7:M:73:VAL:HG22	2.00	0.42
8:P:142:ALA:HA	8:P:145:ILE:HG22	2.00	0.42
9:a:129:LYS:HE2	9:a:129:LYS:HB3	1.89	0.42
9:a:484:MET:O	9:a:488:TYR:HB3	2.19	0.42
9:a:527:THR:HG23	12:e:67:GLN:NE2	2.33	0.42
19:b:304:POV:H14	13:s:417:ALA:HB3	1.58	0.42
2:D:59:ILE:HG23	2:D:95:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:116:LEU:HD21	5:K:144:VAL:HG12	2.02	0.42
9:a:37:PHE:HA	9:a:323:VAL:HG12	2.02	0.42
13:s:403:PHE:O	13:s:404:ASN:ND2	2.52	0.42
16:f:79:LEU:HA	16:f:82:PHE:HB2	2.00	0.42
2:E:335:TYR:HE2	2:E:369:THR:HG22	1.85	0.42
2:F:270:GLU:O	2:F:274:THR:OG1	2.35	0.42
3:G:62:ASP:OD2	3:G:301:ARG:NH1	2.53	0.42
4:H:145:LEU:CD1	6:L:89:LEU:HD22	2.49	0.42
5:J:155:TYR:CD2	5:J:163:VAL:CG1	3.02	0.42
9:a:168:LEU:HD23	9:a:168:LEU:HA	1.91	0.42
13:s:454:PHE:HB3	15:q:46:VAL:HG21	2.01	0.42
15:p:82:ASP:OD1	15:p:82:ASP:N	2.50	0.42
1:A:338:ARG:HG3	1:A:404:VAL:HG23	2.01	0.42
1:B:25:SER:O	1:B:25:SER:OG	2.34	0.42
2:E:307:LEU:HD23	2:E:327:MET:HG3	2.02	0.42
4:H:71:GLU:OE2	4:H:130:GLN:HG2	2.20	0.42
5:J:148:VAL:O	5:J:152:ILE:HG13	2.19	0.42
8:P:197:ARG:HB3	8:P:238:MET:HE1	2.02	0.42
11:d:122:ILE:HD13	11:d:142:ASN:HB3	2.01	0.42
15:m:147:ILE:HD11	15:m:70:LEU:HD21	2.01	0.42
1:B:149:GLY:HA3	1:B:170:PRO:HA	2.00	0.42
1:B:167:MET:HE3	1:B:167:MET:HB2	1.92	0.42
2:F:498:SER:O	2:F:501:SER:OG	2.38	0.42
3:G:10:PRO:HD2	3:G:310:TYR:CZ	2.53	0.42
9:a:595:TRP:CH2	12:e:58:ALA:HB2	2.54	0.42
11:d:208:MET:HE2	11:d:208:MET:HB2	1.89	0.42
15:p:148:VAL:HG11	15:q:23:MET:HG2	2.02	0.42
1:C:217:VAL:HA	1:C:395:LEU:HG	2.02	0.42
2:D:208:ARG:HD2	2:D:251:ASN:OD1	2.19	0.42
2:F:54:ASN:OD1	2:F:54:ASN:N	2.50	0.42
8:P:300:LEU:HA	8:P:303:LEU:HB2	2.02	0.42
9:a:482:ARG:NH1	12:e:77:ARG:HG2	2.34	0.42
12:e:24:GLY:H	12:e:25:PRO:HD2	1.84	0.42
15:g:23:MET:HE3	15:g:27:ALA:HB2	2.02	0.42
15:o:16:VAL:HG12	15:o:17:MET:HE2	2.02	0.42
1:B:258:VAL:CG1	1:B:287:VAL:HG22	2.49	0.42
1:B:267:SER:O	1:B:269:SER:N	2.53	0.42
2:D:108:LYS:HA	2:D:108:LYS:HD3	1.88	0.42
4:H:133:LYS:O	4:H:137:ASN:ND2	2.52	0.42
8:P:289:LEU:HD23	8:P:289:LEU:HA	1.91	0.42
9:a:442:THR:HG21	15:n:53:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:56:LEU:HD23	10:b:56:LEU:HA	1.87	0.42
19:b:301:POV:H15B	13:s:330:TYR:CZ	2.55	0.42
1:A:534:PHE:CE1	1:A:537:THR:CB	2.98	0.42
1:B:372:SER:HB3	1:B:420:PRO:HG2	2.01	0.42
1:C:416:ASP:OD2	1:C:418:SER:OG	2.35	0.42
2:D:445:THR:HG23	2:D:448:ASP:H	1.85	0.42
3:G:116:GLN:NE2	3:G:120:ASN:H	2.18	0.42
5:K:73:SER:O	5:K:77:ASN:N	2.46	0.42
9:a:369:LYS:NZ	9:a:448:TYR:OH	2.53	0.42
9:a:482:ARG:CB	9:a:482:ARG:HH11	2.31	0.42
13:s:263:THR:HG21	13:s:408:LYS:HA	2.02	0.42
15:m:61:MET:HE1	15:m:136:ILE:HD13	2.01	0.42
1:C:220:LYS:HA	1:C:392:VAL:HG23	2.01	0.42
5:J:121:LEU:HD13	5:J:151:ALA:HB1	2.00	0.42
9:a:599:ASN:HA	12:e:62:PRO:O	2.20	0.42
19:b:304:POV:H14A	19:b:304:POV:H11A	1.81	0.42
11:d:320:LYS:HA	11:d:320:LYS:HD3	1.89	0.42
1:A:41:GLU:HB3	1:A:54:ILE:HD12	2.02	0.42
1:A:217:VAL:HA	1:A:395:LEU:HG	2.02	0.42
1:A:534:PHE:HE1	1:A:537:THR:CB	2.30	0.42
1:B:519:PHE:HB2	1:B:544:MET:HE1	2.02	0.42
1:C:138:CYS:C	1:C:140:ASN:N	2.77	0.42
1:C:305:ILE:O	1:C:309:THR:OG1	2.33	0.42
2:F:268:THR:HA	2:F:271:ARG:HG3	2.02	0.42
8:P:329:GLN:CA	8:P:332:SER:HB3	2.39	0.42
9:a:179:ARG:HD3	9:a:179:ARG:HA	1.86	0.42
9:a:481:VAL:CG1	9:a:510:VAL:HG12	2.22	0.42
11:d:263:GLN:HA	11:d:266:ASN:HD21	1.85	0.42
13:s:435:LEU:HD13	19:p:201:POV:H312	2.02	0.42
1:A:22:HIS:O	1:A:22:HIS:ND1	2.54	0.41
1:B:338:ARG:HG3	1:B:404:VAL:HG23	2.02	0.41
1:C:37:ALA:HB2	1:C:81:ARG:HH11	1.84	0.41
2:F:298:THR:HA	2:F:299:ASP:HA	1.80	0.41
5:K:221:ASN:OD1	5:K:221:ASN:N	2.46	0.41
6:L:67:ASN:HA	6:L:91:ILE:O	2.20	0.41
9:a:415:LEU:HD11	16:f:21:TRP:HE1	1.84	0.41
9:a:481:VAL:CG1	9:a:510:VAL:HG22	2.47	0.41
13:s:364:ILE:H	13:s:364:ILE:HG13	1.68	0.41
15:n:34:THR:HG23	15:n:59:VAL:HG13	2.01	0.41
1:B:211:VAL:HG23	1:B:212:ARG:HD2	2.03	0.41
1:C:152:ILE:HD13	1:C:165:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:LEU:HA	1:C:608:MET:HE2	2.02	0.41
5:K:127:LEU:HD23	5:K:132:MET:HG2	2.02	0.41
9:a:224:PHE:HD1	9:a:226:GLY:H	1.68	0.41
9:a:652:LEU:HG	9:a:725:THR:HG21	2.02	0.41
1:A:270:ASP:HB2	1:A:342:TYR:HB3	2.01	0.41
1:A:431:VAL:HG23	1:A:457:TYR:CE2	2.55	0.41
1:A:507:ILE:HD13	1:A:555:VAL:HG21	2.03	0.41
1:C:25:SER:O	1:C:25:SER:OG	2.38	0.41
2:D:506:ARG:HA	2:D:506:ARG:HD2	1.79	0.41
2:F:172:THR:OG1	2:F:178:ASP:OD1	2.35	0.41
2:F:414:ASP:OD2	2:F:481:TRP:NE1	2.39	0.41
3:G:38:PHE:HB3	3:G:320:LEU:HB2	2.02	0.41
8:P:400:VAL:HG13	8:P:407:LYS:HG2	2.02	0.41
15:q:140:VAL:O	15:q:144:TYR:N	2.49	0.41
1:B:368:MET:HA	1:B:369:PRO:HD3	1.87	0.41
5:K:152:ILE:H	5:K:153:PRO:HD2	1.85	0.41
5:K:208:MET:HA	5:K:211:VAL:HG22	2.02	0.41
7:O:111:HIS:HA	7:O:112:PRO:HD3	1.77	0.41
9:a:506:ALA:HB3	9:a:600:ALA:HB3	2.01	0.41
9:a:516:PRO:HB3	12:e:9:PRO:HB3	2.03	0.41
1:B:324:GLU:HA	1:B:354:TRP:HE1	1.85	0.41
1:B:387:GLU:HG3	2:D:264:ALA:HB3	2.03	0.41
2:E:363:HIS:HB3	2:E:366:PRO:HD2	2.02	0.41
7:O:107:ARG:HA	7:O:108:PRO:HD2	1.42	0.41
9:a:385:THR:HG22	9:a:820:GLY:H	1.85	0.41
9:a:496:ARG:HE	12:e:70:ASN:ND2	2.08	0.41
9:a:550:LEU:HD23	9:a:580:MET:HE2	2.03	0.41
10:b:200:ARG:HH12	15:c:78:ASN:HA	1.85	0.41
19:b:305:POV:O14	13:s:419:PHE:N	2.52	0.41
13:s:314:LEU:HB3	13:s:315:PHE:H	1.69	0.41
13:s:345:ILE:CD1	13:s:393:MET:HE3	2.18	0.41
15:l:45:SER:HB2	15:l:52:ILE:HD11	2.02	0.41
1:B:258:VAL:HG11	1:B:287:VAL:HG22	2.02	0.41
2:F:102:THR:HG22	2:F:105:ILE:HD12	2.02	0.41
7:N:111:HIS:O	7:N:113:ASN:N	2.54	0.41
13:s:283:LEU:HD11	13:s:314:LEU:HD21	2.03	0.41
13:s:448:LEU:HD21	15:p:112:ILE:HG13	2.03	0.41
15:m:33:GLY:O	15:m:37:SER:OG	2.33	0.41
15:n:77:ALA:HA	15:n:80:LEU:HD12	2.02	0.41
1:A:505:ASP:O	1:A:508:THR:OG1	2.29	0.41
1:B:266:TYR:CB	1:B:531:PHE:CE1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TRP:HB2	1:C:205:MET:HE1	2.01	0.41
1:C:381:ARG:HA	1:C:381:ARG:HD3	1.95	0.41
1:C:570:ILE:HG23	1:C:574:MET:HG3	2.03	0.41
8:P:276:GLU:OE1	8:P:319:PHE:CZ	2.70	0.41
9:a:482:ARG:N	9:a:483:PRO:HD2	2.36	0.41
13:s:274:VAL:HG11	13:s:321:PHE:HE1	1.86	0.41
15:o:148:VAL:HG11	15:p:23:MET:HG2	2.03	0.41
3:G:150:LEU:HD13	3:G:272:LYS:HD2	2.01	0.41
5:I:116:LEU:HD21	5:I:144:VAL:HG12	2.03	0.41
9:a:31:GLU:OE1	9:a:299:LYS:NZ	2.41	0.41
9:a:97:LEU:HD23	9:a:97:LEU:HA	1.93	0.41
10:b:19:LEU:HA	10:b:19:LEU:HD22	1.46	0.41
10:b:54:ILE:HG21	15:q:152:LEU:HD21	2.03	0.41
13:s:310:THR:HG23	13:s:320:THR:HB	2.01	0.41
13:s:362:PRO:HG2	13:s:365:TYR:HD2	1.86	0.41
1:A:526:THR:HG23	1:A:526:THR:O	2.21	0.41
1:B:526:THR:HA	1:B:527:PRO:HD3	1.93	0.41
1:B:528:TYR:CE1	1:B:586:PHE:HD1	2.39	0.41
1:B:565:ILE:HG22	1:B:567:TRP:H	1.86	0.41
1:C:43:VAL:HG21	1:C:64:ILE:HD13	2.03	0.41
1:C:66:VAL:HG12	1:C:68:GLU:H	1.84	0.41
2:D:250:GLU:O	2:D:250:GLU:CG	2.69	0.41
3:G:278:PRO:HA	3:G:281:ARG:HG2	2.03	0.41
10:b:111:ILE:HD11	10:b:137:MET:HG2	2.03	0.41
15:k:6:ASN:OD1	15:k:6:ASN:N	2.54	0.41
15:p:127:LEU:O	15:p:131:MET:N	2.49	0.41
1:C:371:ASP:OD1	1:C:371:ASP:N	2.53	0.41
2:D:234:MET:N	2:D:298:THR:O	2.48	0.41
3:G:262:LYS:HE3	3:G:262:LYS:HB3	1.92	0.41
8:P:67:GLN:O	8:P:69:GLU:N	2.54	0.41
12:e:41:LEU:HA	12:e:41:LEU:HD13	1.36	0.41
13:s:368:HIS:ND1	13:s:398:PHE:O	2.54	0.41
1:B:148:THR:OG1	1:B:149:GLY:N	2.54	0.40
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.80	0.40
1:B:507:ILE:HD12	1:B:507:ILE:HA	1.96	0.40
1:C:232:ARG:NH1	1:C:518:ASP:O	2.55	0.40
5:J:222:ARG:HG2	5:J:223:LYS:HG3	2.02	0.40
11:d:138:MET:O	11:d:138:MET:HG3	2.21	0.40
11:d:190:LEU:HD23	11:d:190:LEU:HA	1.95	0.40
5:I:183:ILE:HG23	5:I:192:VAL:HB	2.03	0.40
5:J:163:VAL:HB	5:J:165:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:528:ASN:O	9:a:531:THR:CG2	2.62	0.40
9:a:575:PRO:HB3	9:a:650:TRP:HE3	1.86	0.40
1:A:305:ILE:HD12	1:A:305:ILE:HA	2.00	0.40
1:A:526:THR:CG2	1:A:526:THR:O	2.69	0.40
2:F:285:LEU:HA	2:F:289:CYS:HB2	2.03	0.40
1:A:318:MET:HE2	1:A:318:MET:HB3	2.00	0.40
1:C:603:GLN:O	1:C:607:ASP:N	2.54	0.40
2:D:272:ILE:HA	2:D:303:TYR:HE1	1.86	0.40
2:F:99:PHE:HB3	2:F:270:GLU:HG2	2.02	0.40
2:F:124:SER:OG	2:F:125:GLU:N	2.54	0.40
4:H:69:LEU:HD13	4:H:134:LEU:HD21	1.95	0.40
8:P:240:GLU:OE2	8:P:280:GLU:OE1	2.39	0.40
9:a:482:ARG:CB	9:a:482:ARG:CZ	2.98	0.40
1:C:169:PRO:HA	1:C:170:PRO:HD3	1.89	0.40
2:D:166:PRO:HA	2:D:340:ARG:HD3	2.03	0.40
2:E:175:SER:OG	2:E:462:PHE:O	2.30	0.40
5:J:89:ASP:HA	5:J:92:THR:HG22	2.02	0.40
11:d:137:GLN:O	11:d:138:MET:CG	2.50	0.40
13:s:362:PRO:O	13:s:362:PRO:CG	2.62	0.40
15:k:22:ALA:HB2	15:k:96:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	585/617 (95%)	566 (97%)	18 (3%)	1 (0%)	43 70
1	B	586/617 (95%)	562 (96%)	19 (3%)	5 (1%)	14 41
1	C	595/617 (96%)	583 (98%)	12 (2%)	0	100 100
2	D	457/511 (89%)	442 (97%)	14 (3%)	1 (0%)	43 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	454/511 (89%)	436 (96%)	17 (4%)	1 (0%)	43	70
2	F	455/511 (89%)	443 (97%)	12 (3%)	0	100	100
3	G	338/382 (88%)	326 (96%)	11 (3%)	1 (0%)	36	64
4	H	209/247 (85%)	204 (98%)	5 (2%)	0	100	100
5	I	216/226 (96%)	211 (98%)	5 (2%)	0	100	100
5	J	216/226 (96%)	212 (98%)	4 (2%)	0	100	100
5	K	218/226 (96%)	212 (97%)	6 (3%)	0	100	100
6	L	101/119 (85%)	92 (91%)	6 (6%)	3 (3%)	3	18
7	M	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	14	41
7	N	106/118 (90%)	105 (99%)	1 (1%)	0	100	100
7	O	106/118 (90%)	101 (95%)	3 (3%)	2 (2%)	6	25
8	P	364/465 (78%)	342 (94%)	20 (6%)	2 (0%)	24	53
9	a	744/838 (89%)	704 (95%)	37 (5%)	3 (0%)	30	58
10	b	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
11	d	346/351 (99%)	329 (95%)	16 (5%)	1 (0%)	36	64
12	e	71/81 (88%)	63 (89%)	8 (11%)	0	100	100
13	s	203/468 (43%)	177 (87%)	25 (12%)	1 (0%)	24	53
14	r	44/351 (12%)	39 (89%)	5 (11%)	0	100	100
15	c	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	k	148/155 (96%)	148 (100%)	0	0	100	100
15	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	o	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
15	p	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
15	q	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
16	f	41/98 (42%)	40 (98%)	1 (2%)	0	100	100
All	All	8098/9416 (86%)	7811 (96%)	265 (3%)	22 (0%)	37	64

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	268	ASN
1	B	588	ASP
2	E	390	PRO
6	L	96	HIS
6	L	97	PRO
6	L	99	ASP
8	P	68	THR
8	P	370	TYR
9	a	7	SER
1	A	140	ASN
9	a	499	PRO
13	s	349	GLY
1	B	592	ASP
3	G	179	SER
7	O	110	VAL
7	O	112	PRO
1	B	589	PRO
7	M	108	PRO
2	D	136	GLY
9	a	482	ARG
11	d	91	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/524 (95%)	491 (99%)	6 (1%)	63	72
1	B	500/524 (95%)	497 (99%)	3 (1%)	78	80
1	C	504/524 (96%)	502 (100%)	2 (0%)	84	82
2	D	394/432 (91%)	392 (100%)	2 (0%)	81	80
2	E	391/432 (90%)	391 (100%)	0	100	100
2	F	392/432 (91%)	391 (100%)	1 (0%)	86	84
3	G	313/344 (91%)	313 (100%)	0	100	100
4	H	182/212 (86%)	180 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	150/198 (76%)	149 (99%)	1 (1%)	76	78
5	J	153/198 (77%)	152 (99%)	1 (1%)	76	78
5	K	144/198 (73%)	143 (99%)	1 (1%)	76	78
6	L	89/100 (89%)	87 (98%)	2 (2%)	45	63
7	M	38/97 (39%)	38 (100%)	0	100	100
7	N	38/97 (39%)	38 (100%)	0	100	100
7	O	38/97 (39%)	37 (97%)	1 (3%)	40	61
8	P	275/415 (66%)	273 (99%)	2 (1%)	76	78
9	a	667/744 (90%)	660 (99%)	7 (1%)	68	75
10	b	156/158 (99%)	155 (99%)	1 (1%)	78	80
11	d	303/306 (99%)	302 (100%)	1 (0%)	86	84
12	e	62/68 (91%)	60 (97%)	2 (3%)	34	59
13	s	184/398 (46%)	182 (99%)	2 (1%)	65	74
14	r	42/315 (13%)	42 (100%)	0	100	100
15	c	106/110 (96%)	106 (100%)	0	100	100
15	g	106/110 (96%)	105 (99%)	1 (1%)	70	76
15	k	106/110 (96%)	105 (99%)	1 (1%)	70	76
15	l	106/110 (96%)	106 (100%)	0	100	100
15	m	106/110 (96%)	106 (100%)	0	100	100
15	n	106/110 (96%)	106 (100%)	0	100	100
15	o	107/110 (97%)	107 (100%)	0	100	100
15	p	107/110 (97%)	107 (100%)	0	100	100
15	q	107/110 (97%)	107 (100%)	0	100	100
16	f	38/84 (45%)	38 (100%)	0	100	100
All	All	6507/7887 (82%)	6468 (99%)	39 (1%)	76	80

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	122	VAL
1	A	462	ASP
1	A	463	GLU
1	A	526	THR

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Mol	Chain	Res	Type
1	A	534	PHE
1	B	141	LEU
1	B	560	GLN
1	B	587	LYS
1	C	199	ILE
1	C	470	THR
2	D	250	GLU
2	D	251	ASN
2	F	379	VAL
4	H	75	THR
4	H	101	VAL
5	I	163	VAL
5	J	154	VAL
5	K	154	VAL
6	L	10	VAL
6	L	39	VAL
7	O	113	ASN
8	P	296	VAL
8	P	366	ASN
9	a	88	VAL
9	a	377	ILE
9	a	465	ASN
9	a	482	ARG
9	a	496	ARG
9	a	756	LEU
9	a	776	LEU
10	b	19	LEU
11	d	276	LEU
12	e	59	GLN
12	e	74	TRP
13	s	270	GLN
13	s	425	TRP
15	g	59	VAL
15	k	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	140	ASN
1	A	159	ASN
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	314	ASN
1	A	397	ASN
1	A	603	GLN
1	A	609	GLN
1	A	610	ASN
1	B	65	GLN
1	B	314	ASN
1	B	397	ASN
1	B	430	GLN
1	B	468	HIS
1	B	523	ASN
1	B	610	ASN
1	C	22	HIS
1	C	114	GLN
1	C	159	ASN
1	C	213	GLN
1	C	397	ASN
1	C	522	GLN
2	D	205	GLN
2	D	237	ASN
2	D	482	GLN
2	E	62	HIS
2	E	171	GLN
2	E	237	ASN
2	E	384	HIS
2	E	385	ASN
2	E	465	GLN
2	E	482	GLN
2	F	38	ASN
2	F	42	GLN
2	F	226	ASN
2	F	251	ASN
2	F	262	ASN
2	F	265	ASN
2	F	288	GLN
2	F	358	ASN
2	F	384	HIS
2	F	385	ASN
2	F	420	ASN
2	F	433	GLN
2	F	465	GLN

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Mol	Chain	Res	Type
2	F	482	GLN
3	G	30	ASN
3	G	39	ASN
3	G	88	GLN
3	G	134	ASN
3	G	226	ASN
3	G	239	HIS
3	G	275	GLN
3	G	315	ASN
4	H	113	HIS
4	H	130	GLN
5	I	122	GLN
5	I	206	GLN
5	J	77	ASN
5	J	122	GLN
5	J	149	GLN
5	J	194	ASN
5	K	63	GLN
5	K	67	GLN
5	K	100	GLN
6	L	54	GLN
6	L	57	ASN
6	L	96	HIS
7	M	109	GLN
7	M	113	ASN
7	N	109	GLN
7	O	88	GLN
7	O	89	GLN
7	O	91	ASN
7	O	113	ASN
8	P	222	GLN
8	P	273	ASN
8	P	299	GLN
8	P	305	GLN
8	P	417	GLN
9	a	53	ASN
9	a	76	ASN
9	a	85	ASN
9	a	199	GLN
9	a	269	GLN
9	a	280	GLN
9	a	365	ASN

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Mol	Chain	Res	Type
9	a	375	GLN
9	a	412	HIS
9	a	534	ASN
9	a	548	HIS
9	a	612	HIS
9	a	720	HIS
9	a	721	GLN
9	a	735	ASN
9	a	751	GLN
9	a	802	HIS
9	a	812	GLN
10	b	128	HIS
10	b	148	ASN
11	d	145	GLN
11	d	165	GLN
11	d	171	GLN
11	d	243	HIS
11	d	254	GLN
11	d	266	ASN
12	e	67	GLN
12	e	70	ASN
13	s	270	GLN
13	s	327	ASN
13	s	336	HIS
13	s	358	GLN
13	s	404	ASN
15	c	78	ASN
15	c	124	GLN
15	g	78	ASN
15	g	92	GLN
15	g	123	GLN
15	g	124	GLN
15	k	6	ASN
15	k	78	ASN
15	k	92	GLN
15	l	78	ASN
15	l	92	GLN
15	l	124	GLN
15	m	78	ASN
15	m	123	GLN
15	n	78	ASN
15	n	81	ASN

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Mol	Chain	Res	Type
15	n	123	GLN
15	n	124	GLN
15	o	124	GLN
15	p	78	ASN
15	p	92	GLN
15	p	124	GLN
15	q	78	ASN
15	q	81	ASN
15	q	92	GLN
15	q	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	POV	b	302	-	46,46,51	1.03	4 (8%)	52,54,59	0.93	2 (3%)
19	POV	p	201	-	43,43,51	1.07	3 (6%)	49,51,59	0.93	3 (6%)
19	POV	r	402	-	46,46,51	1.03	3 (6%)	52,54,59	0.86	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ADP	C	702	17	28,29,29	0.93	1 (3%)	43,45,45	1.88	9 (20%)
19	POV	b	304	-	46,46,51	1.03	4 (8%)	52,54,59	0.91	2 (3%)
20	NAG	s	503	13	14,14,15	0.43	0	17,19,21	0.57	0
20	NAG	s	501	13	14,14,15	0.35	0	17,19,21	0.48	0
20	NAG	s	504	13	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
19	POV	b	305	-	30,30,51	1.27	4 (13%)	36,38,59	0.99	2 (5%)
21	OLA	r	403	-	19,19,19	0.79	1 (5%)	19,19,19	0.90	0
19	POV	g	201	-	42,42,51	1.07	2 (4%)	48,50,59	0.95	2 (4%)
20	NAG	s	502	13	14,14,15	0.36	0	17,19,21	0.53	0
20	NAG	s	505	13	14,14,15	0.20	0	17,19,21	0.60	0
20	NAG	s	506	-	14,14,15	0.28	0	19,19,21	0.31	0
19	POV	r	401	-	46,46,51	1.01	4 (8%)	52,54,59	0.84	2 (3%)
19	POV	b	301	-	46,46,51	1.02	4 (8%)	52,54,59	0.94	2 (3%)
19	POV	b	303	-	40,40,51	1.10	4 (10%)	46,48,59	0.92	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	POV	b	302	-	-	24/50/50/55	-
19	POV	p	201	-	-	19/47/47/55	-
19	POV	r	402	-	-	29/50/50/55	-
18	ADP	C	702	17	-	1/16/32/32	0/3/3/3
19	POV	b	304	-	-	27/50/50/55	-
20	NAG	s	503	13	-	2/6/23/26	0/1/1/1
20	NAG	s	501	13	-	0/6/23/26	0/1/1/1
20	NAG	s	504	13	-	0/6/23/26	0/1/1/1
19	POV	b	305	-	-	19/34/34/55	-
21	OLA	r	403	-	-	9/17/17/17	-
19	POV	g	201	-	-	22/46/46/55	-
20	NAG	s	502	13	-	2/6/23/26	0/1/1/1
20	NAG	s	505	13	-	1/6/23/26	0/1/1/1
20	NAG	s	506	-	-	1/6/22/26	0/1/1/1
19	POV	r	401	-	-	24/50/50/55	-
19	POV	b	301	-	-	30/50/50/55	-
19	POV	b	303	-	-	23/44/44/55	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	p	201	POV	O21-C2	-3.10	1.39	1.46
19	b	305	POV	O21-C2	-2.91	1.39	1.46
19	g	201	POV	O21-C2	-2.90	1.39	1.46
19	r	402	POV	O21-C2	-2.89	1.39	1.46
19	b	304	POV	O21-C2	-2.76	1.40	1.46
19	b	303	POV	O21-C2	-2.75	1.40	1.46
21	r	403	OLA	C10-C9	2.74	1.47	1.31
19	b	302	POV	O21-C2	-2.71	1.40	1.46
19	b	304	POV	O31-C3	-2.57	1.39	1.45
19	g	201	POV	O31-C31	2.52	1.40	1.33
19	b	302	POV	O31-C31	2.48	1.40	1.33
19	r	401	POV	O21-C21	2.46	1.41	1.34
19	r	401	POV	O31-C31	2.44	1.40	1.33
19	b	301	POV	O31-C31	2.38	1.40	1.33
19	p	201	POV	O31-C31	2.38	1.40	1.33
19	b	305	POV	O31-C3	-2.37	1.39	1.45
19	b	301	POV	O21-C21	2.36	1.40	1.34
19	b	303	POV	O31-C31	2.35	1.40	1.33
19	r	402	POV	O31-C31	2.31	1.40	1.33
19	b	303	POV	O31-C3	-2.31	1.40	1.45
18	C	702	ADP	PA-O3A	2.28	1.62	1.59
19	r	402	POV	O31-C3	-2.26	1.40	1.45
19	b	304	POV	O31-C31	2.26	1.39	1.33
19	b	305	POV	O31-C31	2.25	1.39	1.33
19	p	201	POV	O31-C3	-2.24	1.40	1.45
19	b	301	POV	O31-C3	-2.22	1.40	1.45
19	r	401	POV	O31-C3	-2.22	1.40	1.45
19	r	401	POV	O21-C2	-2.19	1.41	1.46
19	b	302	POV	O21-C21	2.15	1.40	1.34
19	b	301	POV	O21-C2	-2.13	1.41	1.46
19	b	302	POV	O31-C3	-2.13	1.40	1.45
19	b	304	POV	O21-C21	2.12	1.40	1.34
19	b	305	POV	O21-C21	2.10	1.40	1.34
19	b	303	POV	O21-C21	2.08	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	702	ADP	C5-C4-N3	-5.75	118.80	126.72
18	C	702	ADP	N3-C4-N9	4.70	135.15	127.17
19	b	302	POV	O21-C21-C22	4.55	121.31	111.48
18	C	702	ADP	N3-C2-N1	-4.28	122.10	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	304	POV	O21-C21-C22	4.13	120.42	111.48
19	b	301	POV	O21-C21-C22	3.95	120.02	111.48
19	g	201	POV	O21-C21-C22	3.88	119.88	111.48
18	C	702	ADP	C5-N7-C8	3.84	109.48	103.45
18	C	702	ADP	C2-N3-C4	3.80	121.10	111.83
19	b	305	POV	O21-C21-C22	3.72	119.53	111.48
19	b	303	POV	O21-C21-C22	3.71	119.51	111.48
19	r	401	POV	O21-C21-C22	3.71	119.50	111.48
19	r	402	POV	O21-C21-C22	3.61	119.30	111.48
19	p	201	POV	O21-C21-C22	3.60	119.27	111.48
18	C	702	ADP	C4-C5-N7	-3.11	107.03	110.58
19	g	201	POV	O31-C31-C32	2.96	120.85	111.83
19	b	301	POV	O31-C31-C32	2.93	120.77	111.83
20	s	504	NAG	C1-O5-C5	2.81	115.96	112.19
18	C	702	ADP	N9-C8-N7	-2.69	110.12	113.94
19	b	302	POV	O31-C31-C32	2.65	119.92	111.83
19	p	201	POV	O31-C31-C32	2.61	119.80	111.83
19	b	303	POV	O31-C31-C32	2.55	119.60	111.83
19	r	402	POV	O31-C31-C32	2.53	119.55	111.83
19	r	401	POV	O31-C31-C32	2.52	119.50	111.83
19	b	305	POV	O31-C31-C32	2.49	119.42	111.83
19	p	201	POV	C2-O21-C21	-2.46	111.90	117.80
18	C	702	ADP	O3B-PB-O3A	2.38	112.62	104.64
19	b	304	POV	O31-C31-C32	2.34	118.98	111.83
18	C	702	ADP	PA-O5'-C5'	-2.06	109.53	121.35

There are no chirality outliers.

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	b	301	POV	C1-O11-P-O12
19	b	301	POV	C1-O11-P-O14
19	b	301	POV	C11-O12-P-O11
19	b	301	POV	C11-O12-P-O13
19	b	301	POV	C3-C2-O21-C21
19	b	301	POV	C22-C21-O21-C2
19	b	302	POV	C1-O11-P-O12
19	b	302	POV	C1-O11-P-O14
19	b	302	POV	C11-O12-P-O11
19	b	302	POV	C11-O12-P-O13
19	b	302	POV	C11-O12-P-O14
19	b	302	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
19	b	302	POV	C22-C21-O21-C2
19	b	303	POV	C11-O12-P-O14
19	b	304	POV	C1-O11-P-O14
19	b	304	POV	O22-C21-O21-C2
19	b	305	POV	C1-O11-P-O13
19	r	401	POV	C11-O12-P-O11
19	r	401	POV	C11-O12-P-O14
19	r	401	POV	C22-C21-O21-C2
19	r	402	POV	C11-O12-P-O11
19	r	402	POV	C11-O12-P-O13
19	r	402	POV	O12-C11-C12-N
19	g	201	POV	C11-O12-P-O11
19	g	201	POV	O12-C11-C12-N
19	g	201	POV	C22-C21-O21-C2
19	p	201	POV	C1-O11-P-O12
19	p	201	POV	C1-O11-P-O13
19	p	201	POV	C11-O12-P-O11
19	b	301	POV	O32-C31-O31-C3
19	b	301	POV	C32-C31-O31-C3
19	b	301	POV	O22-C21-O21-C2
19	r	401	POV	O22-C21-O21-C2
19	b	304	POV	C22-C21-O21-C2
19	b	302	POV	O22-C21-O21-C2
19	g	201	POV	O22-C21-O21-C2
20	s	503	NAG	O5-C5-C6-O6
20	s	502	NAG	O5-C5-C6-O6
21	r	403	OLA	C11-C10-C9-C8
19	p	201	POV	C22-C23-C24-C25
19	r	402	POV	C32-C31-O31-C3
19	r	402	POV	O32-C31-O31-C3
19	b	304	POV	C33-C34-C35-C36
20	s	503	NAG	C4-C5-C6-O6
19	p	201	POV	C22-C21-O21-C2
20	s	502	NAG	C4-C5-C6-O6
19	b	301	POV	C31-C32-C33-C34
19	b	303	POV	C31-C32-C33-C34
19	b	304	POV	C21-C22-C23-C24
19	r	401	POV	C21-C22-C23-C24
21	r	403	OLA	C1-C2-C3-C4
19	g	201	POV	C21-C22-C23-C24
20	s	506	NAG	O5-C5-C6-O6
19	p	201	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
19	r	402	POV	O21-C2-C3-O31
20	s	505	NAG	O5-C5-C6-O6
19	b	303	POV	C35-C36-C37-C38
21	r	403	OLA	C11-C12-C13-C14
19	b	303	POV	C22-C21-O21-C2
19	b	305	POV	C31-C32-C33-C34
19	b	305	POV	C22-C23-C24-C25
19	r	401	POV	C22-C23-C24-C25
19	b	301	POV	C37-C38-C39-C310
19	p	201	POV	C35-C36-C37-C38
19	p	201	POV	C23-C24-C25-C26
19	b	301	POV	C33-C34-C35-C36
19	b	302	POV	C24-C25-C26-C27
19	b	305	POV	C22-C21-O21-C2
19	r	402	POV	C210-C211-C212-C213
19	b	304	POV	C32-C31-O31-C3
19	r	401	POV	C39-C310-C311-C312
19	r	401	POV	C34-C35-C36-C37
19	b	304	POV	C23-C24-C25-C26
19	b	301	POV	C23-C24-C25-C26
19	r	402	POV	C22-C21-O21-C2
19	b	303	POV	O22-C21-O21-C2
19	b	301	POV	C210-C211-C212-C213
19	b	301	POV	C26-C27-C28-C29
19	b	302	POV	C21-C22-C23-C24
19	r	402	POV	C35-C36-C37-C38
19	b	303	POV	C36-C37-C38-C39
19	r	401	POV	C31-C32-C33-C34
19	r	402	POV	C21-C22-C23-C24
19	r	402	POV	O22-C21-O21-C2
19	r	401	POV	C36-C37-C38-C39
19	b	304	POV	O32-C31-O31-C3
19	b	304	POV	C34-C35-C36-C37
19	g	201	POV	C31-C32-C33-C34
19	r	402	POV	C26-C27-C28-C29
19	b	302	POV	C23-C24-C25-C26
19	r	402	POV	C39-C310-C311-C312
19	b	303	POV	C33-C34-C35-C36
19	b	304	POV	C25-C26-C27-C28
19	r	401	POV	C32-C33-C34-C35
19	b	302	POV	C310-C311-C312-C313
19	g	201	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	b	304	POV	C26-C27-C28-C29
19	b	304	POV	O11-C1-C2-C3
19	g	201	POV	O11-C1-C2-C3
19	b	301	POV	C39-C310-C311-C312
19	r	401	POV	C37-C38-C39-C310
19	b	305	POV	O22-C21-O21-C2
19	b	305	POV	C1-C2-C3-O31
19	b	303	POV	C23-C24-C25-C26
19	b	303	POV	C26-C27-C28-C29
19	r	402	POV	C22-C23-C24-C25
19	g	201	POV	C39-C310-C311-C312
19	r	401	POV	C32-C31-O31-C3
19	b	302	POV	C32-C33-C34-C35
19	b	301	POV	C32-C33-C34-C35
19	b	305	POV	C33-C34-C35-C36
19	b	301	POV	C311-C310-C39-C38
19	b	304	POV	C24-C25-C26-C27
19	g	201	POV	C25-C26-C27-C28
19	b	305	POV	C32-C31-O31-C3
19	p	201	POV	C32-C31-O31-C3
19	b	302	POV	C36-C37-C38-C39
19	b	303	POV	O11-C1-C2-C3
19	b	305	POV	O11-C1-C2-C3
19	r	402	POV	O11-C1-C2-C3
19	g	201	POV	C310-C311-C312-C313
19	g	201	POV	C33-C34-C35-C36
21	r	403	OLA	C4-C5-C6-C7
19	b	302	POV	C311-C312-C313-C314
19	b	302	POV	C1-C2-C3-O31
19	b	303	POV	C1-C2-C3-O31
19	r	401	POV	C1-C2-C3-O31
19	r	402	POV	C1-C2-C3-O31
21	r	403	OLA	C2-C3-C4-C5
19	p	201	POV	C24-C25-C26-C27
19	b	304	POV	O11-C1-C2-O21
19	g	201	POV	O11-C1-C2-O21
19	r	402	POV	C25-C26-C27-C28
19	g	201	POV	C311-C312-C313-C314
19	b	305	POV	O21-C2-C3-O31
19	r	401	POV	O21-C2-C3-O31
19	b	301	POV	C35-C36-C37-C38
19	r	401	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
19	r	402	POV	C310-C311-C312-C313
19	g	201	POV	C26-C27-C28-C29
19	b	304	POV	C22-C23-C24-C25
19	b	304	POV	C37-C38-C39-C310
19	b	302	POV	O11-C1-C2-C3
19	p	201	POV	C210-C211-C212-C213
19	b	303	POV	C32-C31-O31-C3
19	p	201	POV	O32-C31-O31-C3
19	b	302	POV	C312-C313-C314-C315
19	b	305	POV	O32-C31-O31-C3
19	p	201	POV	C33-C34-C35-C36
19	r	401	POV	C3-C2-O21-C21
19	b	304	POV	C210-C211-C212-C213
19	b	304	POV	C32-C33-C34-C35
19	r	401	POV	C33-C34-C35-C36
19	b	302	POV	O11-C1-C2-O21
19	p	201	POV	C36-C37-C38-C39
19	g	201	POV	C12-C11-O12-P
19	b	303	POV	O32-C31-O31-C3
19	r	402	POV	C37-C38-C39-C310
19	b	301	POV	O12-C11-C12-N
19	b	302	POV	O12-C11-C12-N
19	b	303	POV	O12-C11-C12-N
19	b	305	POV	O12-C11-C12-N
19	r	401	POV	O12-C11-C12-N
19	p	201	POV	O12-C11-C12-N
19	b	301	POV	C211-C212-C213-C214
19	g	201	POV	C23-C24-C25-C26
19	b	301	POV	C2-C1-O11-P
19	b	303	POV	O11-C1-C2-O21
19	b	305	POV	O11-C1-C2-O21
19	r	402	POV	O11-C1-C2-O21
19	b	301	POV	C29-C210-C211-C212
19	b	301	POV	C27-C28-C29-C210
19	b	301	POV	O21-C2-C3-O31
19	b	303	POV	O21-C2-C3-O31
19	b	304	POV	O21-C2-C3-O31
19	b	301	POV	C1-O11-P-O13
19	b	303	POV	C11-O12-P-O11
19	b	303	POV	C11-O12-P-O13
19	b	305	POV	C1-O11-P-O12
19	b	305	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
19	r	402	POV	C1-O11-P-O12
19	r	402	POV	C1-O11-P-O13
19	r	402	POV	C1-O11-P-O14
19	g	201	POV	C1-O11-P-O14
19	g	201	POV	C11-O12-P-O14
19	p	201	POV	C11-O12-P-O14
19	b	303	POV	C24-C25-C26-C27
19	b	303	POV	C32-C33-C34-C35
19	b	302	POV	C27-C28-C29-C210
21	r	403	OLA	C3-C4-C5-C6
19	r	402	POV	C34-C35-C36-C37
19	g	201	POV	C22-C23-C24-C25
19	r	401	POV	C35-C36-C37-C38
19	b	303	POV	C21-C22-C23-C24
19	b	301	POV	C311-C312-C313-C314
19	b	303	POV	C34-C35-C36-C37
19	g	201	POV	C35-C36-C37-C38
21	r	403	OLA	C6-C7-C8-C9
19	b	304	POV	C310-C311-C312-C313
19	r	401	POV	C29-C210-C211-C212
19	g	201	POV	C27-C28-C29-C210
19	b	304	POV	C29-C210-C211-C212
19	r	402	POV	C27-C28-C29-C210
19	p	201	POV	C29-C210-C211-C212
19	r	402	POV	C33-C34-C35-C36
19	b	302	POV	C39-C310-C311-C312
19	b	304	POV	C27-C28-C29-C210
18	C	702	ADP	PA-O3A-PB-O1B
19	r	401	POV	C312-C313-C314-C315
19	r	401	POV	C27-C28-C29-C210
21	r	403	OLA	C9-C10-C11-C12
19	b	304	POV	C312-C313-C314-C315
19	r	401	POV	C310-C311-C312-C313
19	b	304	POV	C1-C2-C3-O31
21	r	403	OLA	C7-C8-C9-C10
19	b	304	POV	O21-C21-C22-C23
19	b	304	POV	C35-C36-C37-C38
19	b	305	POV	O21-C21-C22-C23
19	b	301	POV	O31-C31-C32-C33
19	b	305	POV	O31-C31-C32-C33
19	r	402	POV	O21-C21-C22-C23
19	b	302	POV	O31-C31-C32-C33

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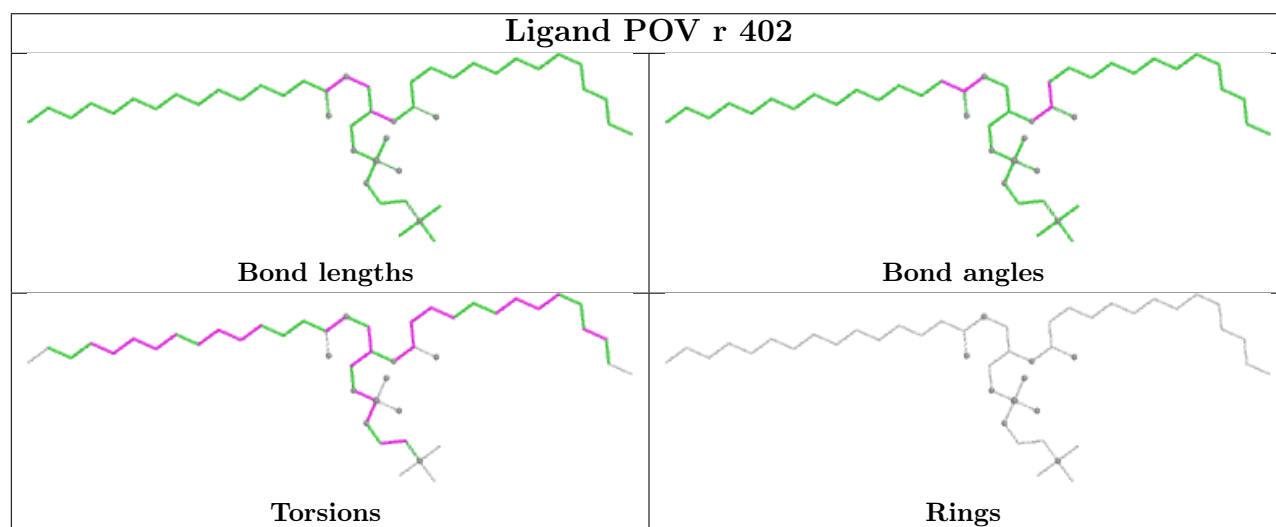
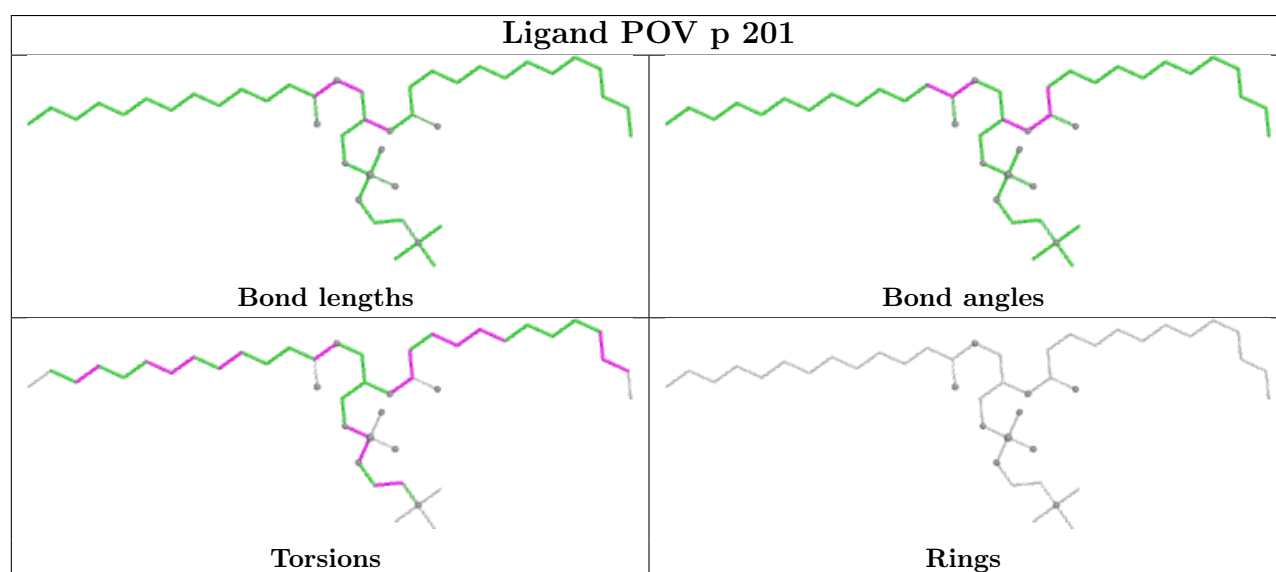
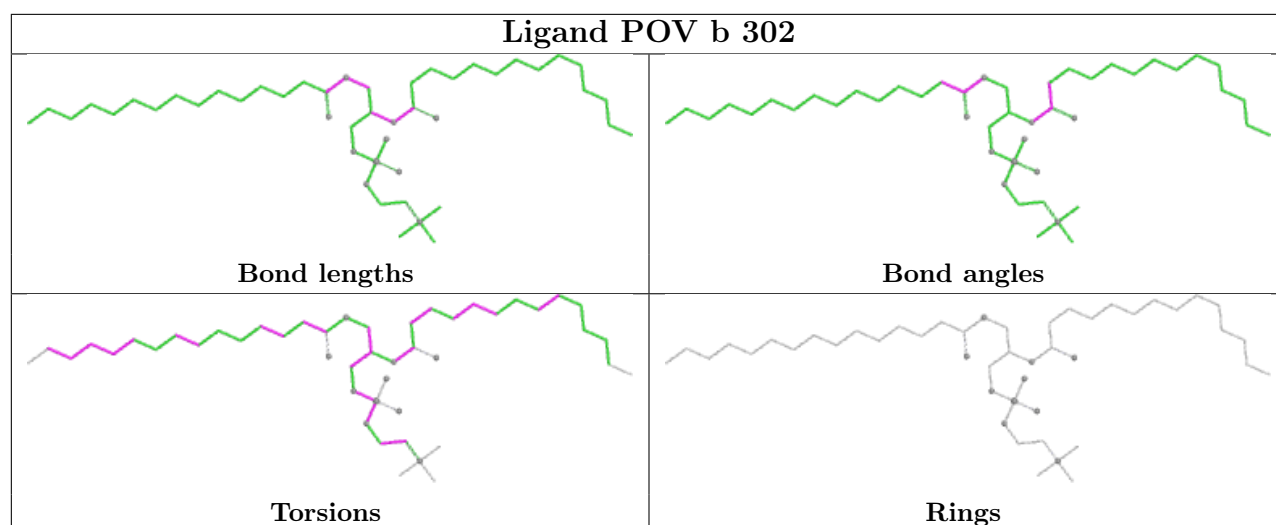
Mol	Chain	Res	Type	Atoms
19	b	304	POV	O22-C21-C22-C23
19	b	302	POV	O32-C31-C32-C33
19	r	402	POV	O22-C21-C22-C23
19	b	305	POV	O32-C31-C32-C33
19	b	301	POV	C1-C2-C3-O31
19	p	201	POV	C39-C310-C311-C312
19	b	305	POV	O22-C21-C22-C23
19	r	402	POV	C311-C310-C39-C38
19	b	303	POV	C29-C210-C211-C212
19	p	201	POV	O21-C21-C22-C23
19	b	301	POV	O32-C31-C32-C33

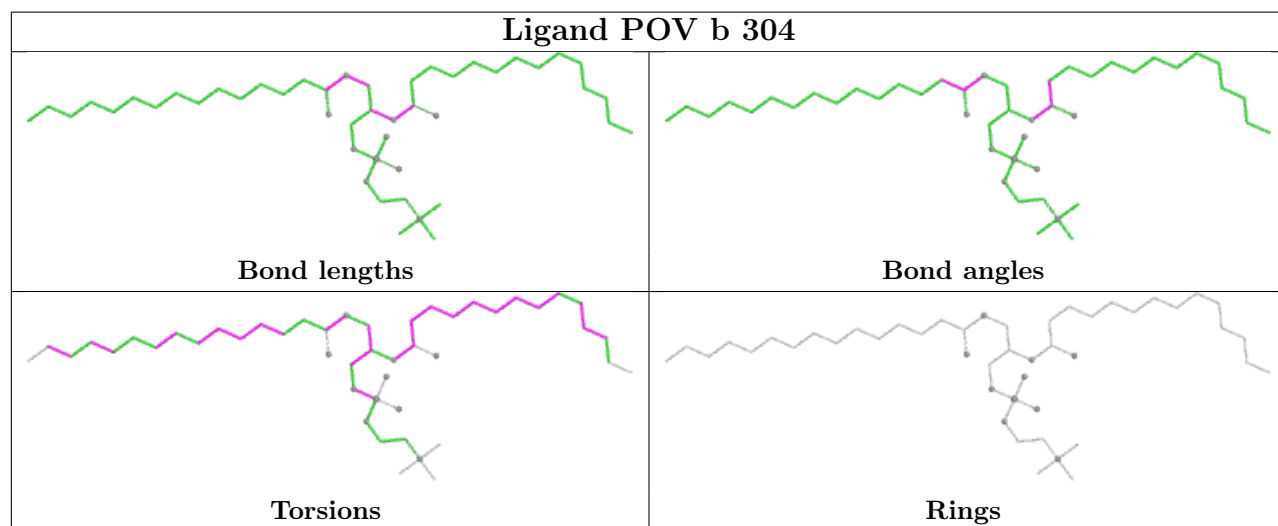
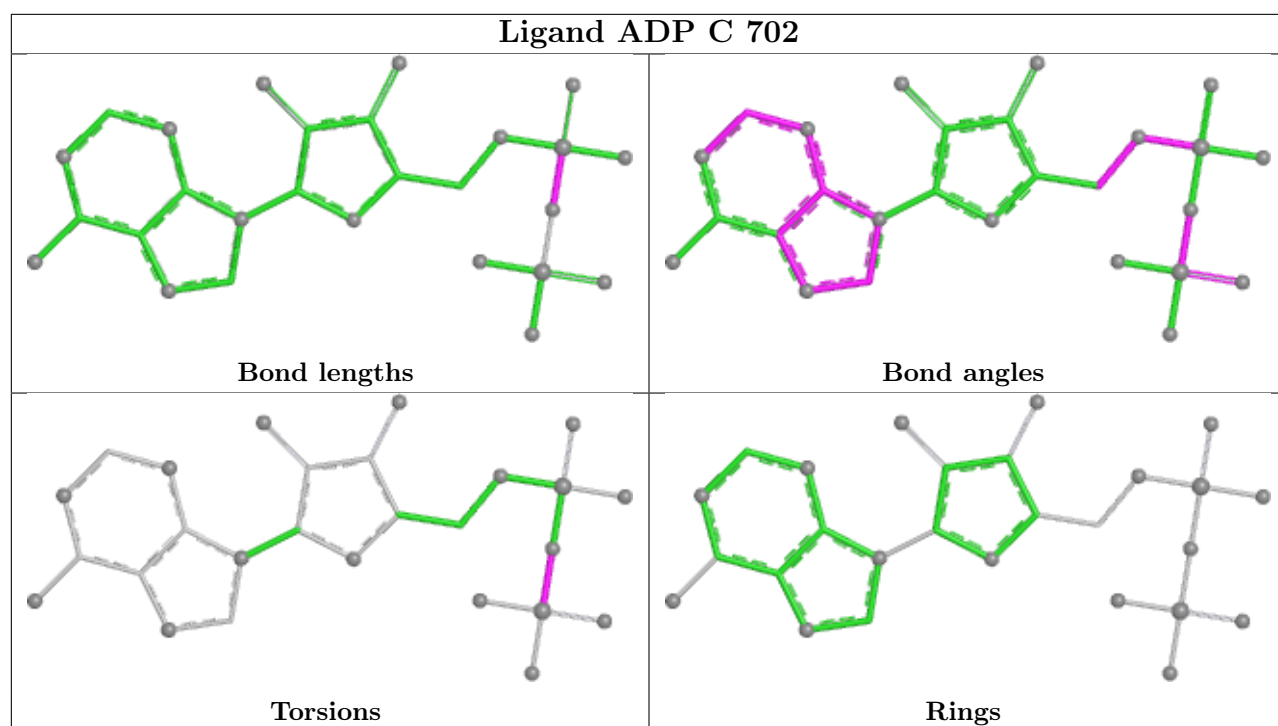
There are no ring outliers.

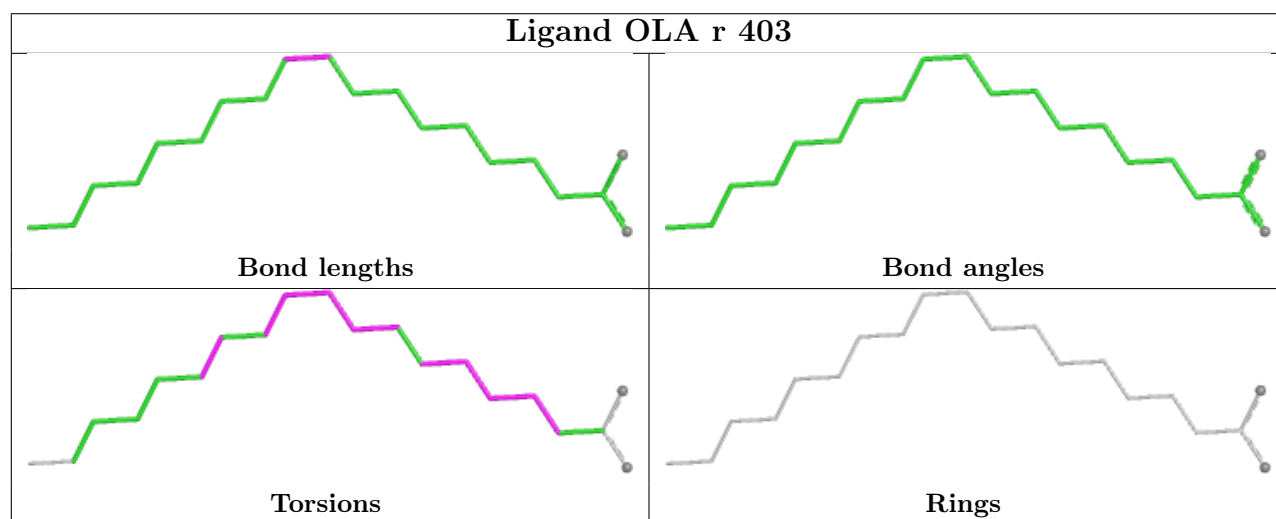
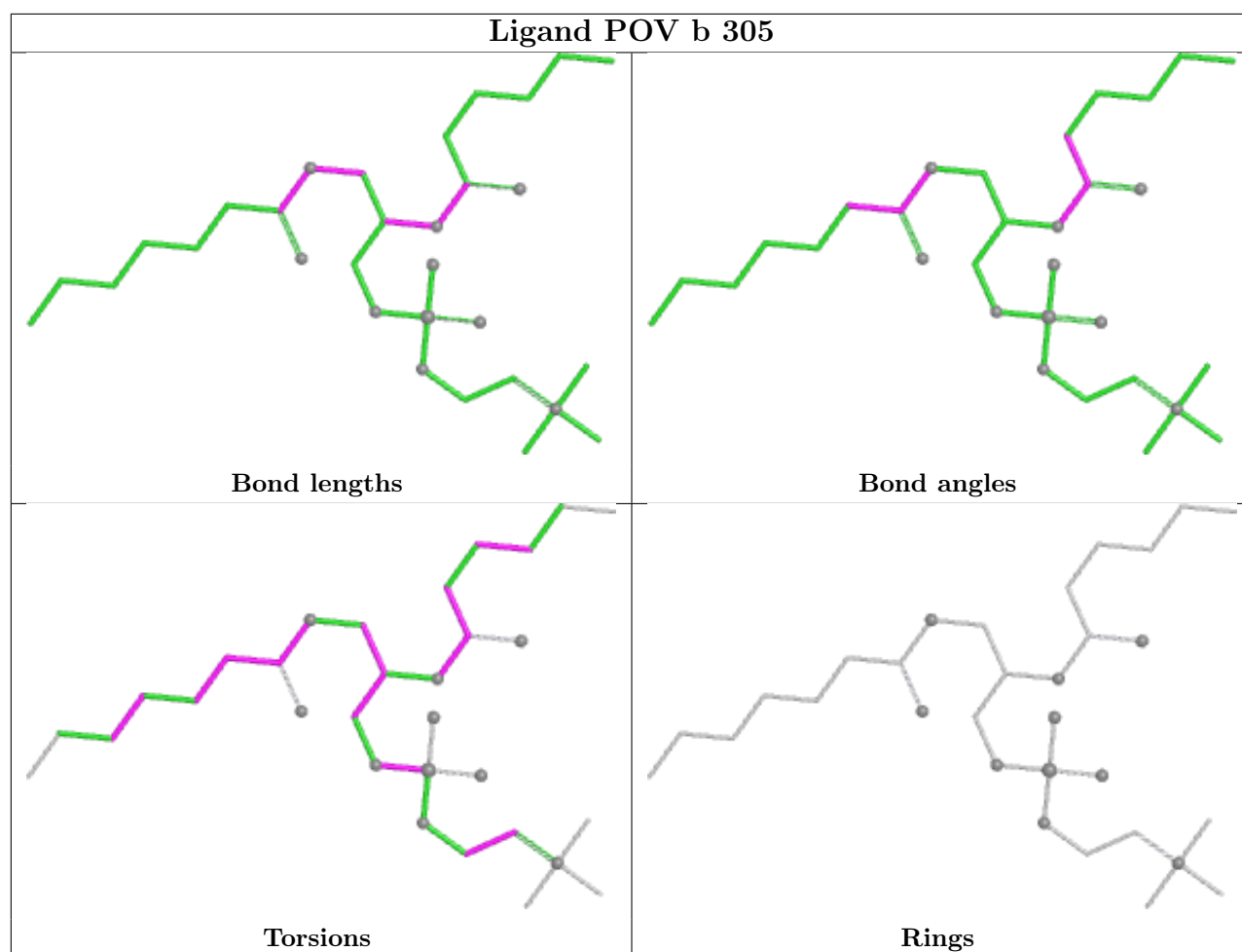
13 monomers are involved in 37 short contacts:

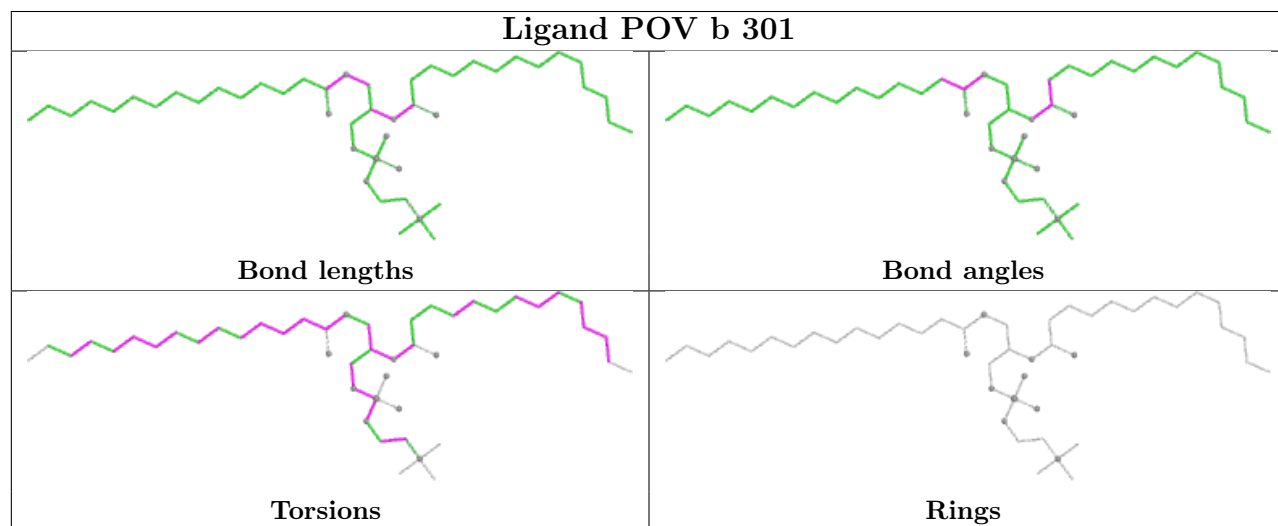
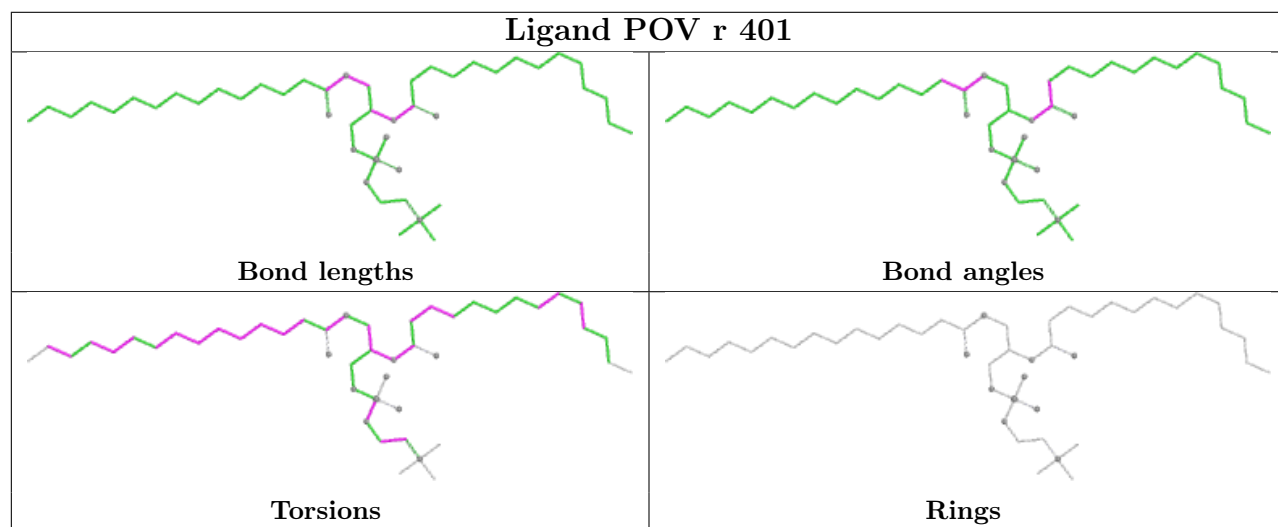
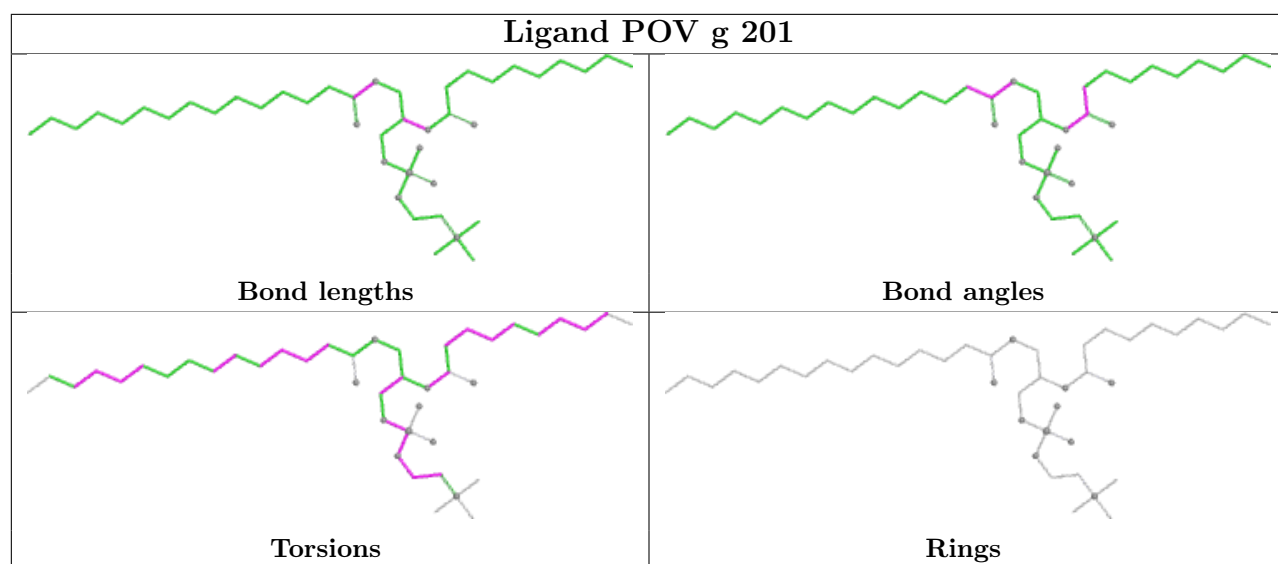
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	p	201	POV	1	0
19	r	402	POV	2	0
18	C	702	ADP	1	0
19	b	304	POV	5	0
20	s	504	NAG	1	0
19	b	305	POV	2	0
21	r	403	OLA	1	0
19	g	201	POV	6	0
20	s	505	NAG	1	0
20	s	506	NAG	9	0
19	r	401	POV	1	0
19	b	301	POV	8	0
19	b	303	POV	1	0

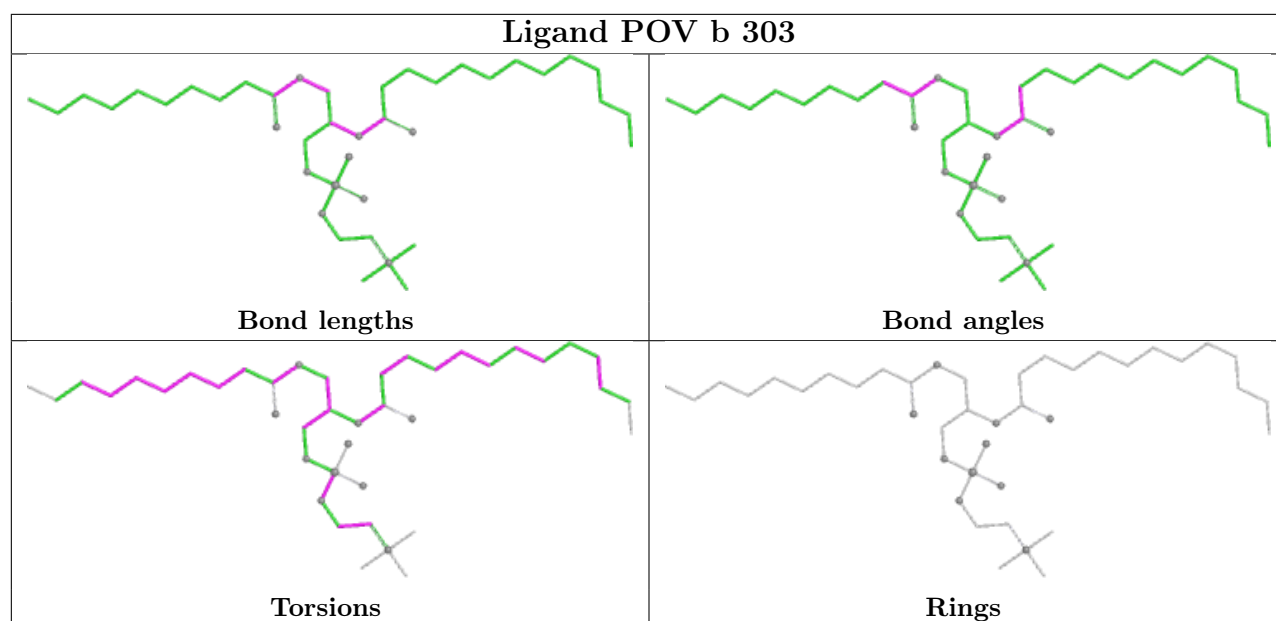
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

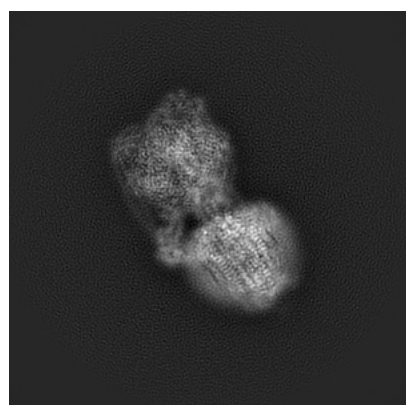
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22121. These allow visual inspection of the internal detail of the map and identification of artifacts.

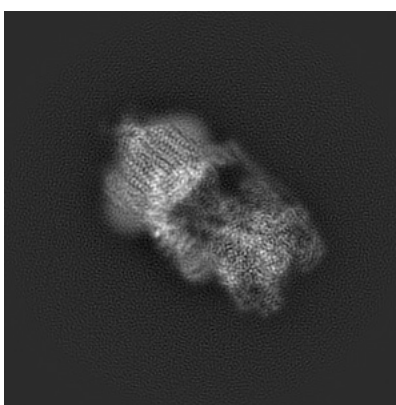
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

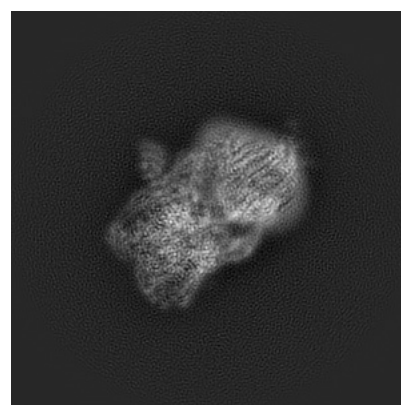
6.1.1 Primary map



X



Y

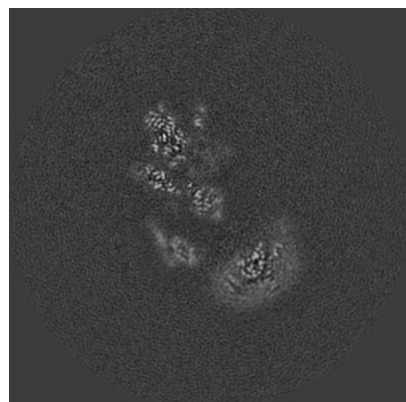


Z

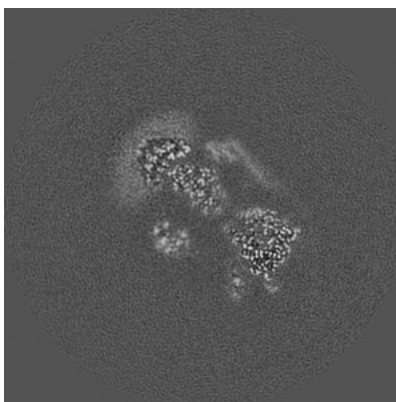
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

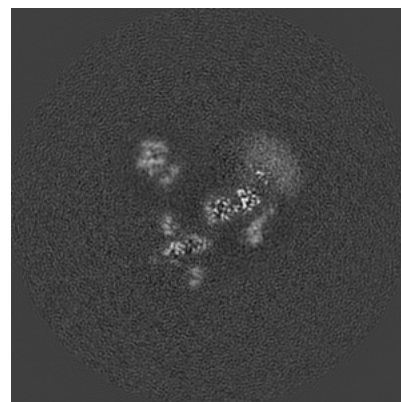
6.2.1 Primary map



X Index: 255



Y Index: 255



Z Index: 255

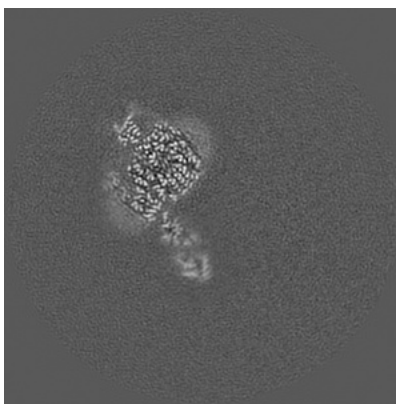
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

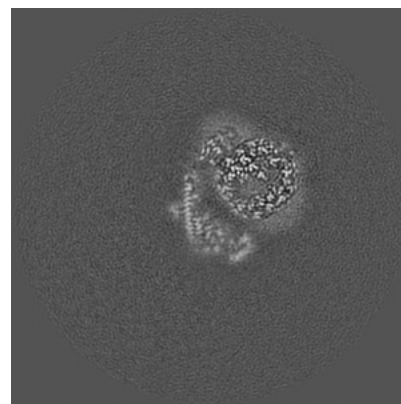
6.3.1 Primary map



X Index: 223



Y Index: 313

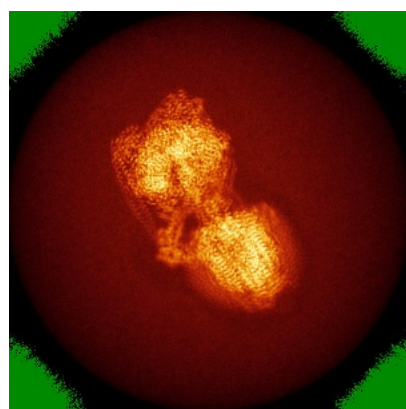


Z Index: 196

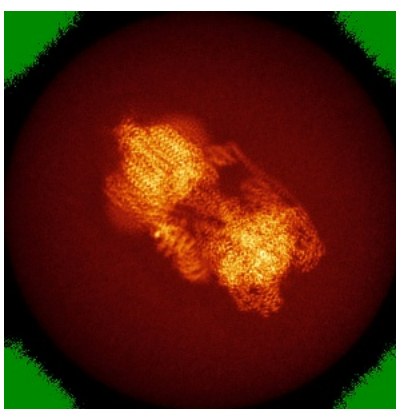
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

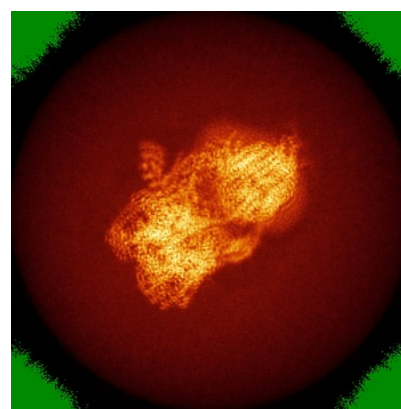
6.4.1 Primary map



X



Y

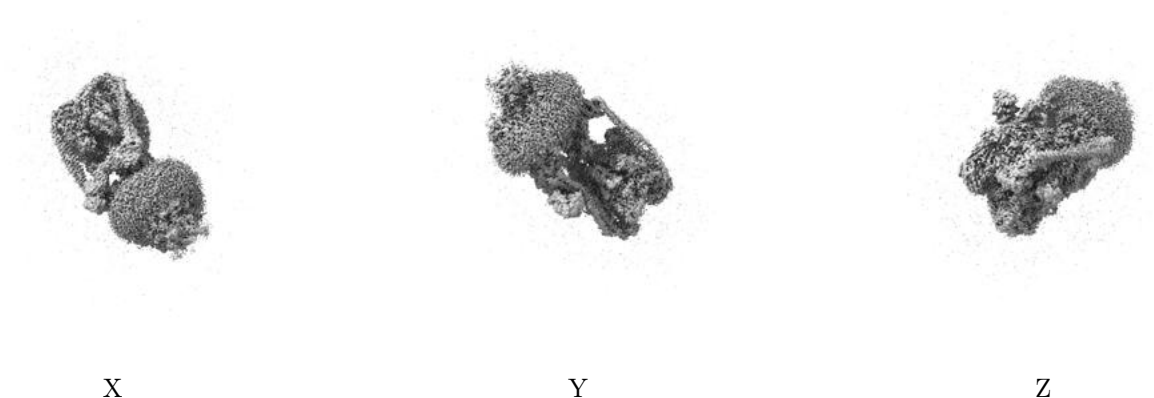


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

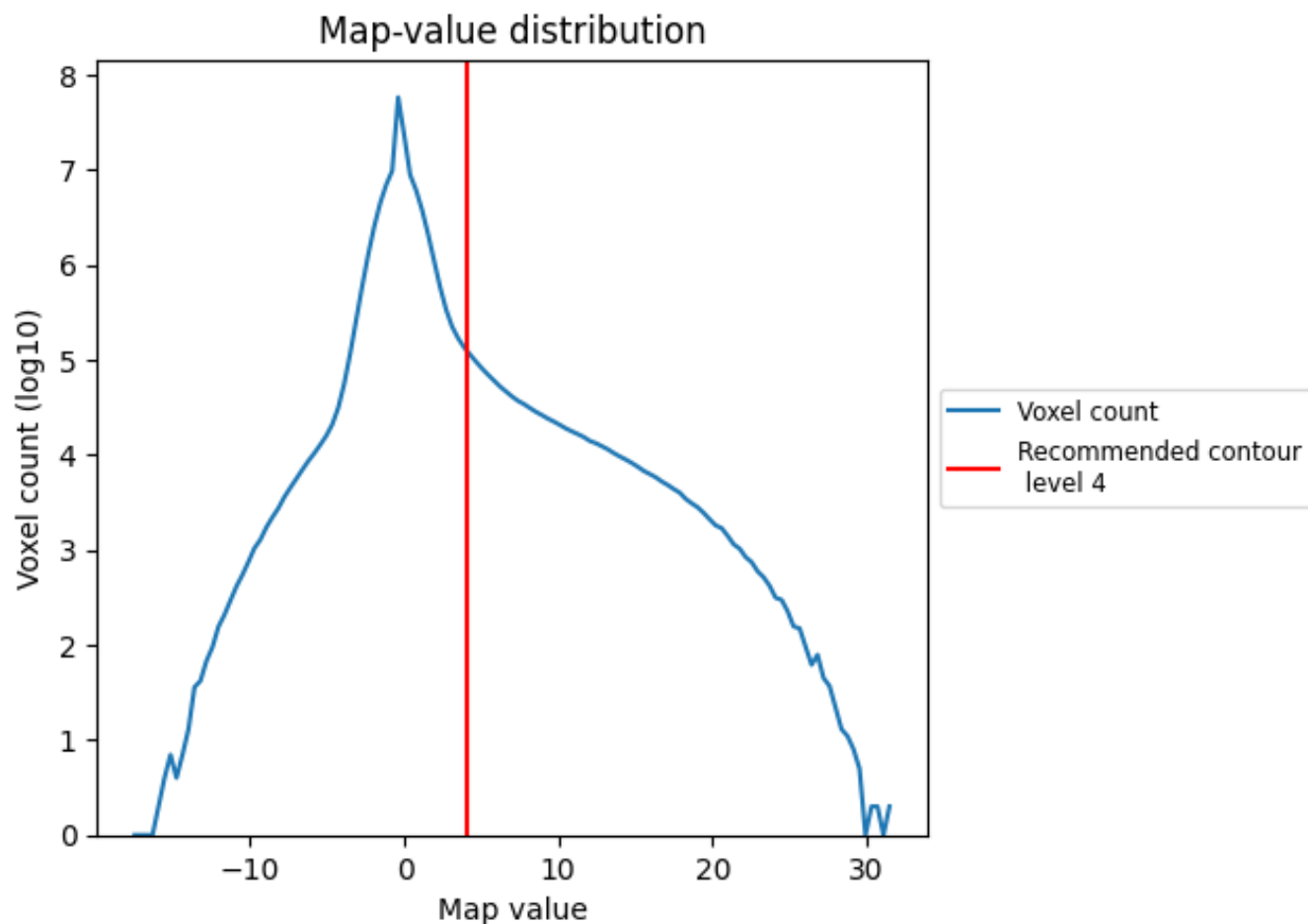
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

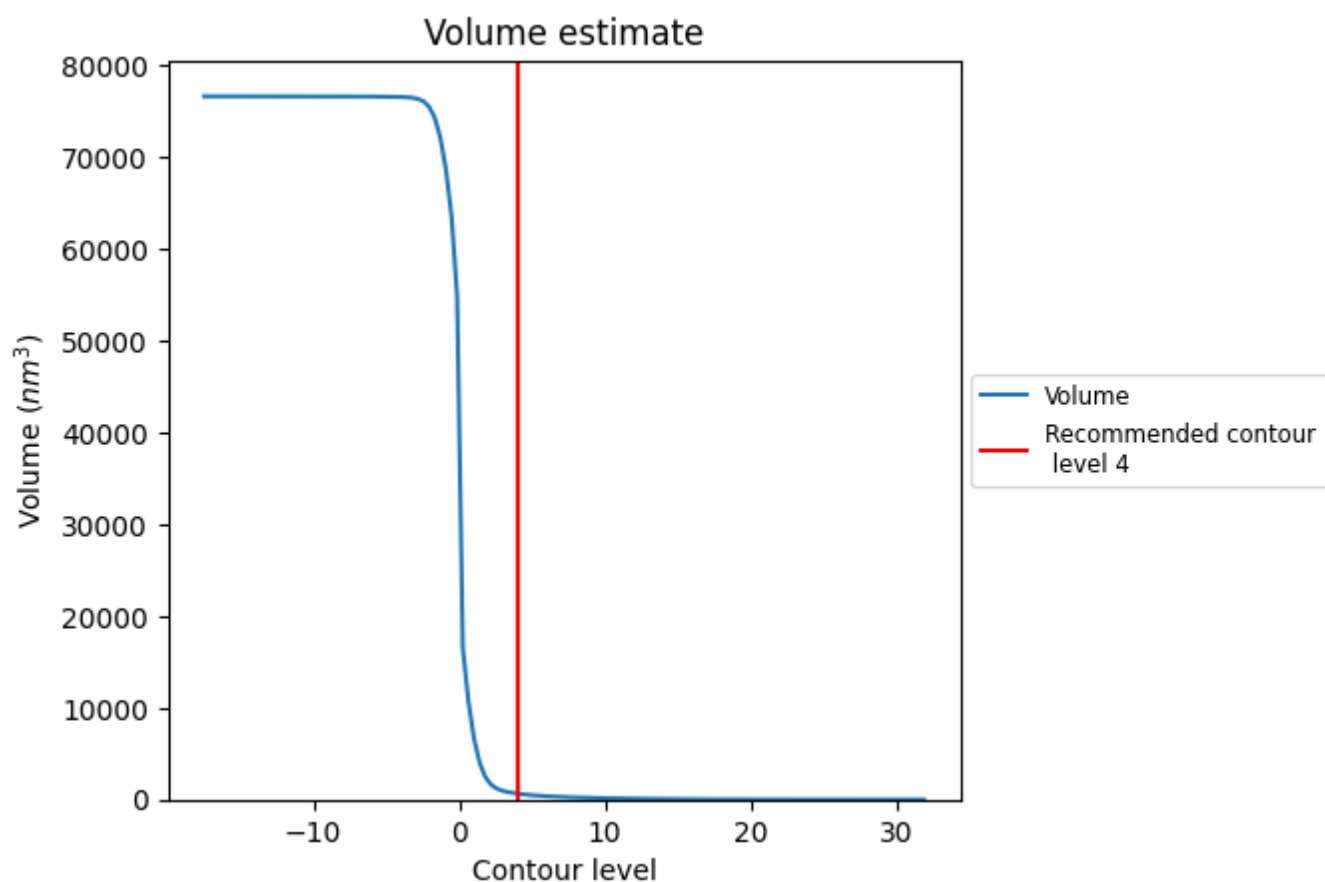
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

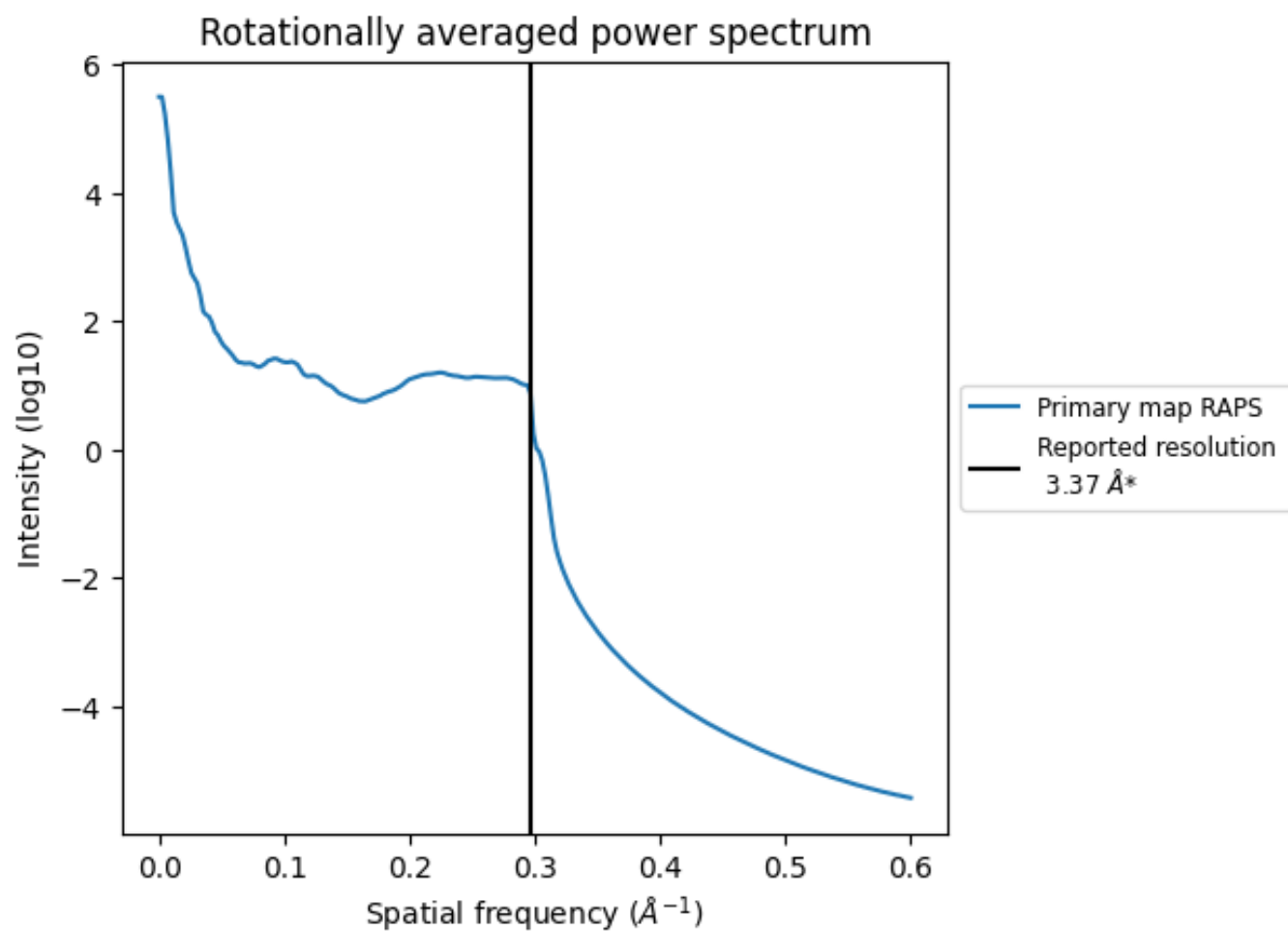
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm³; this corresponds to an approximate mass of 580 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

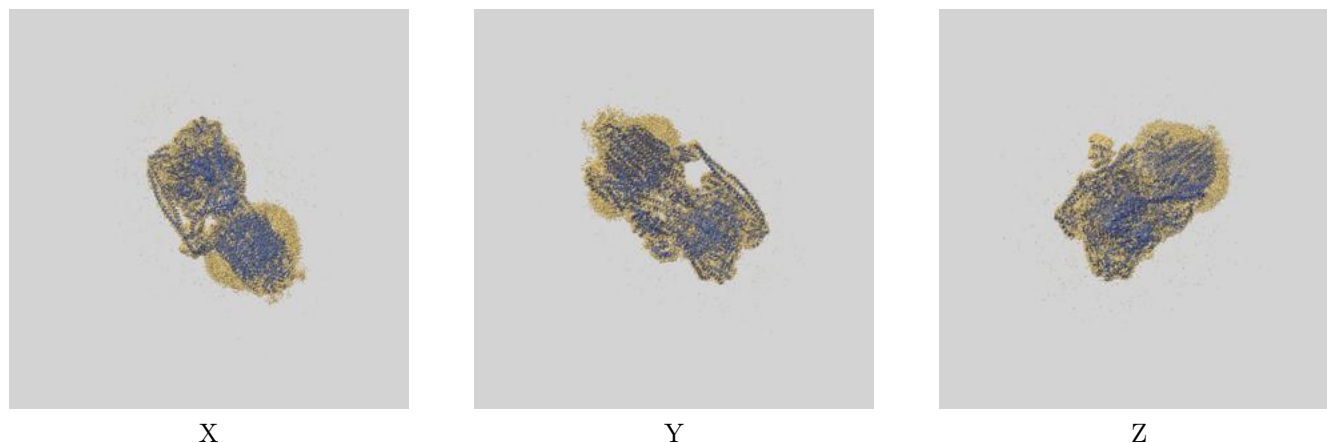
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

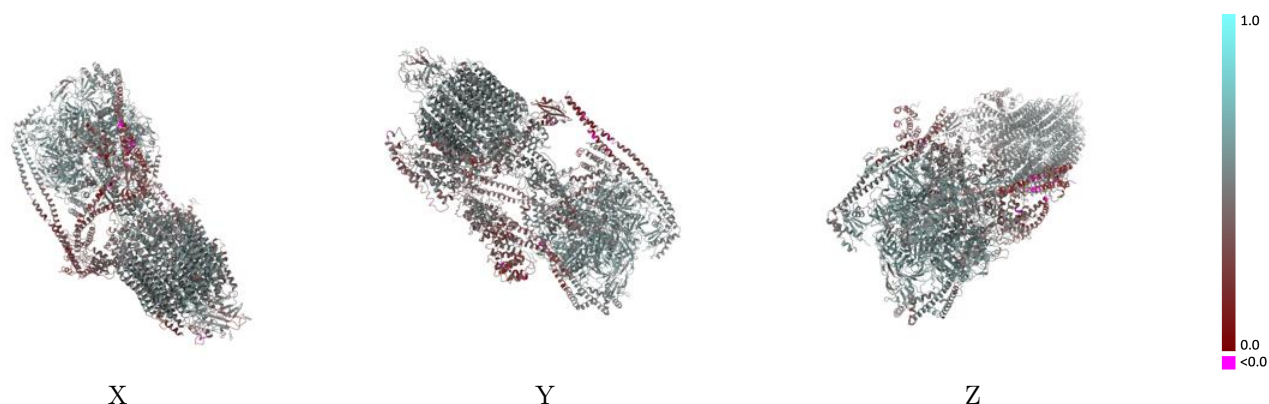
This section contains information regarding the fit between EMDB map EMD-22121 and PDB model 6XBW. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



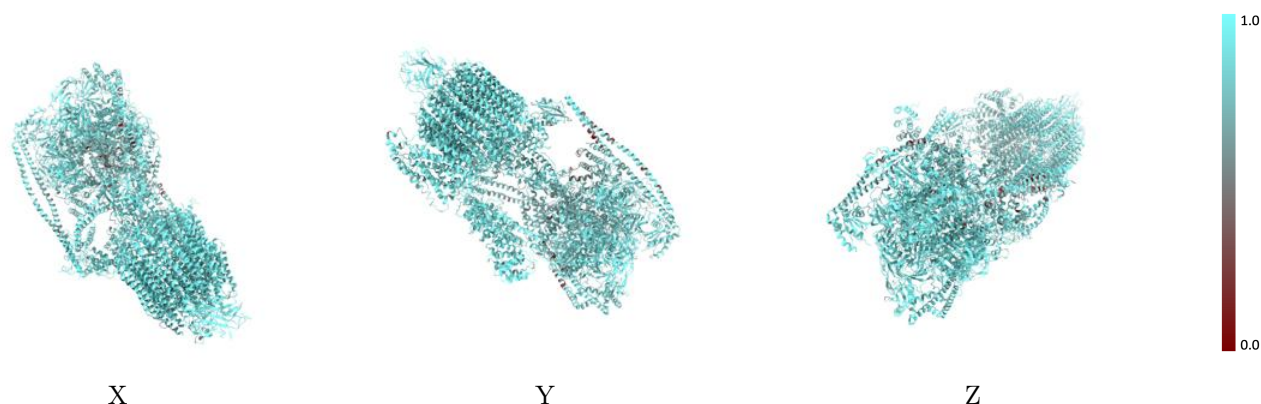
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



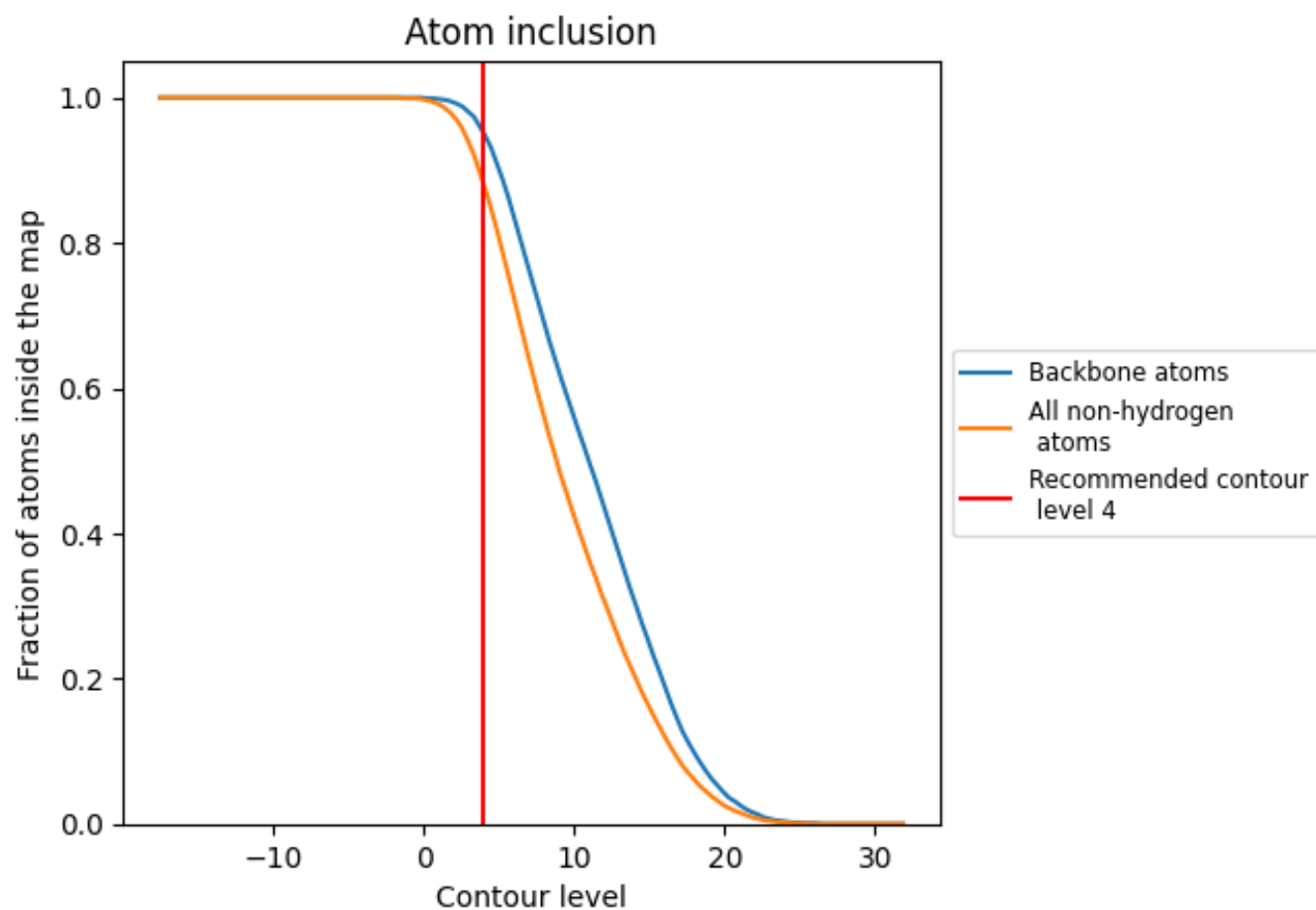
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.4790
A	 0.8470	 0.4920
B	 0.8740	 0.5200
C	 0.8850	 0.5290
D	 0.9130	 0.5510
E	 0.9010	 0.5430
F	 0.8910	 0.5350
G	 0.8340	 0.3010
H	 0.8590	 0.5110
I	 0.8220	 0.4430
J	 0.8560	 0.4680
K	 0.8590	 0.4630
L	 0.8300	 0.4760
M	 0.7720	 0.3570
N	 0.8550	 0.4210
O	 0.7760	 0.3890
P	 0.8550	 0.3310
a	 0.8670	 0.4200
b	 0.9340	 0.5250
c	 0.9300	 0.5180
d	 0.8830	 0.4910
e	 0.8270	 0.3950
f	 0.7930	 0.3270
g	 0.9360	 0.5160
k	 0.9260	 0.5090
l	 0.9280	 0.4980
m	 0.9250	 0.5010
n	 0.9230	 0.5110
o	 0.9390	 0.5170
p	 0.9330	 0.5160
q	 0.9350	 0.5170
r	 0.9310	 0.5360
s	 0.9080	 0.4660

